

**ASSESSMENT OF RISKS ASSOCIATED
WITH CARBON MONOXIDE GAS
DURING WELL PERFORATION**

prepared by:

**Research Triangle Institute
P.O. Box 12194
Research Triangle Park, North Carolina 27709**

for:

**Minerals Management Service
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1.0 Introduction

Carbon monoxide (CO), a toxic, colorless gas, is a well known product of incomplete combustion. It had not been a concern around oil and gas wells until an unexpected and tragic accident occurred at the Seacliff oil well in Ventura County, California in August of 1994 in which three workers were killed due to CO exposure from a well perforation operation. Toxic ambient conditions due to explosive byproducts from perforations at oil wells have apparently been quite rare; however, there are reasons for caution and justification to take appropriate CO safety measures when oil well perforations are taking place.

Perforation is the process of creating holes in the casing of an oil well that penetrate the cement sheath that surrounds the steel casing and extend some depth into the geologic formation through the use of powerful explosives. Perforating allows for fluid flow between the petroleum reservoir and the wellbore.

This report relates information from several types of sources—research, empirical, and theoretical—to the operations at an oil well that contribute to the potential exposure of humans to CO. The goal of RTI's efforts is to provide insights and recommendations for the Mineral Management Service, other governmental bodies, and the petroleum industry to reduce the risks of CO exposure from perforating operations at petroleum sites. For this project, information gathering and analysis have been performed in several areas

- # summary of explosives thermochemistry and the potential for generating CO, Section 2.1.1
- # modeling *CO flux generation* by perforating explosives, Section 2.1.2
- # modeling *CO ambient concentrations* from detonation byproduct release, Section 2.1.3
- # analysis of well perforation practices that may lead to detonation byproduct releases above ground, Section 2.2,
- # review of specific incidents and case studies on explosives use and CO exposure, Section 2.3,
- # review of the health effects of CO and the assessment of risks from exposure to CO from well perforation, Section 3, and

- # review and make recommendations on safety practices to reduce potential CO exposures, Section 4.

Theoretical and research investigations of explosive thermochemistry are well studied and provide ample evidence that CO is generated by detonation of the types of powerful explosives that are used in various industries (e.g., spacecraft launches, mining, oil and gas production, and construction). However, there appears to be a paucity of test information specifically on CO from perforating in the oil industry. Other than the extensive work performed at the national weapons laboratories from which some of this report's conclusions are drawn, there is very little in the published, peer-reviewed literature concerning CO risks from these basic industries. A few case studies are available, and these are reviewed in Section 2.3, Case Studies.

Personnel in the oil completion industry may be unaware that CO is generated during the explosion of such compounds as RDX, HMX, and PETN. General industry safety practices have prevented damaging CO exposures because of safety and health concerns for gases other than CO. At the same time, changes in explosive products, configurations, and perforating operations may be increasing the amount of CO generated. As CO generation information becomes more widely known, reduction of potential CO exposure should follow.

The amount of CO generated by the explosives used in perforation correlates quite closely with the amount of explosives used; CO is a well known product of incomplete combustion, even with the detonation of high explosives. Conditions in the wellbore, such as temperature and pressure, and particularly the presence of fluid, affect the amount of CO generated. Even more importantly, *the explosive molecules are inherently oxygen deficient*. Incomplete combustion due to lack of additional oxygen sources under ground and to quenching of the reactions contribute to the significant volumes of CO. If there is no release of fluids and gases to the atmosphere, CO stays in the wellbore, dissolved in the fluids or imbedded in the geological structures. The potential for release of CO exists where the pressures underground are greater than the hydrostatic pressure in the wellbore (under-balanced condition). Properly carried out oil well safety measures that remove off-gases of any type (e.g., hydrogen sulfide, [H₂S]) are also appropriate for reducing the exposure potential to CO.

Two screening-level modeling efforts were performed as part of this task to help assess the potential health risks of CO associated with oil well perforation. These modeling exercises begin the process of estimating the amounts of CO generated and estimating the concentrations of CO in the vicinity of a release valve where workers could be exposed.

CHEETAH is a computer program developed by the developed by the Lawrence Livermore National Laboratory that estimates amounts of CO resulting from the detonation of specific explosives. It calculates the amounts of all waste gases based on thermochemical theorems, and estimates the explosive gases under conditions simulating above-ground and below-ground explosions. Results from CHEETAH include a "worst-case" (at least in theory) set of combustion gases, where the program converts all the possible carbon and oxygen atoms into CO, rather than a mix of carbon dioxide (CO₂) and CO. Results based on a representative amount of explosive were generated for each of several explosives and for several conditions (Section 2.1.2 and Appendix A). The results are summarized,

based on limited experimental data. However, the worst-case amounts may, in fact, reflect what happens in the “real world.” Researchers have found through calorimetry testing that more CO is generated than was predicted.

Air dispersion models were also used to estimate the concentration of CO downwind from a point release. The CO estimates from CHEETAH were modeled using both an offshore (OCD5) and an onshore (ISC-Prime) model to estimate ambient concentrations from 5 meters to 30 meters from the release point (Section 2.1.3 and Appendix B). Meteorological data from coastal California provided wind speeds and directions that were used in the dispersion models. Again, worst-case conditions (i.e., low wind speed and minimal disturbance) were selected to represent situations with the highest potential exposure levels. Simple assumptions were made as to height, speed, volume, and direction of releases.

Results from both the CHEETAH and ambient air modeling should be viewed as estimates, but they suggest and support the idea that CO is a genuine risk factor at oil well sites where perforation is performed. The likelihood that waste gases from well perforation are released, whether accidentally or deliberately, has not been directly addressed in this task. However, in the event of a release, the modeling performed provides some preliminary estimates of the potential for exposure to dangerous levels of CO.

2.0 Exposure and Consequence Analysis

The three subparts to this section contain the theoretical basis for CO generation, estimates of how much CO is generated, and what are the resulting concentrations of CO in the air surrounding a release. Section, 2.1, Explosives Thermochemistry is the portion of this report that most directly addresses the question of how much CO is generated during well perforation. The modeling results are summarized in Section 2.1 with more detailed modeling results presented in Appendixes A and B.

A review of the physical and engineering basics of oil wells and perforation (Section 2.2) was prepared because the evaluation of CO risks must be considered along with many other factors that the oil industry balances when completing or reusing oil wells. Selection of types of wells, types of perforating guns, and configuration and the conditions of perforations are made to maximize efficiency of operations, all of which influence the amounts of CO generated.

Section 2.3 reviews the available reports of human exposure to byproducts from the detonation of explosives. Although the number of reports is very limited, the information they present concerning CO levels in the environment appears to be consistent with information gathered from field and laboratory research projects and theoretical models.

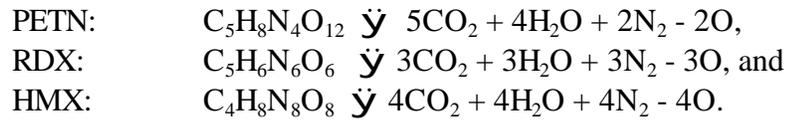
2.1 Explosives Thermochemistry

This section presents an overview of the theoretical bases for predicting the chemical results from explosions, followed by results of modeling specific explosives using CHEETAH, a program that predicts the thermochemical equilibrium for specific explosive products. The output from CHEETAH runs were used to estimate potential CO ambient concentrations, using U.S. Environmental Protection Agency (EPA) models—OCD5 (basic Gaussian dispersion) and ISC-Prime. Sections 2.1.2 and 2.1.3 present the results from CHEETAH and the OCD-ISC modeling.

2.1.1 Science of Explosives

When an explosive reaction takes place, the explosive molecule breaks apart into its constituent atoms. The constituent atoms quickly rearrange themselves into stable molecules, usually water, CO₂, CO, and nitrogen. Other molecules containing carbon, aluminum, and sulfur are found in the products of some explosives. Oxygen is an important determinant of explosive products, and the explosive itself is a source of oxidizing atoms (Akhavan, 1998).

The amount of oxygen with the explosive may or may not be sufficient for complete oxidation of the fuel. Three explosives involved in oil well perforations are PETN, RDX, and HMX, whose balanced reaction formulae for complete combustion are



In all three cases, there is a negative oxygen balance; this means that there is not enough oxygen for all the carbon atoms to be completely oxidized (CO_2). The result is that CO and other (toxic) gases are generated. A large negative oxygen balance inherent to the explosive itself is occurs in oil well perforation, because there are not additional sources of oxygen at the perforation site. On a percentage basis, the oxygen balance for the three primary explosives of interest are

<u>Explosive</u>	<u>Oxygen Balance, %</u>
PETN	-10.13
RDX	-21.60
HMX	-21.62

Percentage oxygen balance is the percentage of total molecular weight contributed by oxygen (O in the above equations).

Both primary and secondary explosives are used for effective detonations (perforations). Primary explosives include lead azide, lead styphnate, and mercury fulminate. PETN, RDX, and HMX and many other explosives, such as nitroglycerine, picric acid, tetryl, and TNT, are defined as secondary explosives.

The explosive process is irreversible and can be diagrammed as

INITIATE

o

EXPLOSION

o

GASEOUS PRODUCT (V) AND HEAT (Q)

Volume of gas (V) and heat of explosion (Q) combine to give a value for explosive power.

$$\text{Explosive Power} = Q \times V$$

The value for explosive power can be compared with the explosive power of a standard explosive (picric acid) resulting in a power index.

$$\text{PowerIndex} = \left(\frac{QV}{Q_{\text{picricacid}} V_{\text{picricacid}}} \right) \times 100$$

The values for power of secondary explosives are much higher than the values for primary explosives, as illustrated in Table 2-1 below.

The volume of gas produced by an explosion is directly related to the amount of work done by the explosive. Detonation gas volumes can be calculated from the equation of decomposition (i.e., the amount of gaseous products liberated). Representative gas volumes at standard temperature and pressure are (Akhavan 1998)

<u>Explosive</u>	<u>Volume of gas, dm³ g⁻¹</u>
PETN	0.780
RDX	0.908
HMX	0.908
Nitroglycerine	0.740
TNT	0.740

Table 2-1. Power Index for Primary and Secondary Explosives

Explosive	Power Index, %
<i>Primary explosives</i>	
Mercury fulminate	14
Lead styphnate	21
Lead azide	13
<i>Secondary explosives</i>	
PETN	167
RDX	169
HMX	168
Nitroglycerine	171
Picric acid	100
TNT	115

The amount of CO generated is a reflection of the oxygen balance, which in turn is related to the heat of explosion. The higher the oxygen balance, the higher the heat of explosion. PETN has a higher heat of explosion (higher oxygen balance) than RDX and HMX, but a lower volume of gas. The resulting power index is nearly identical for all three explosives (power index = 168). As shown and discussed in Section 3.1, the amounts of predicted CO under various conditions varies among the three explosives. HMX appears to generate the least CO, in terms of weight or percentage of total gases, and PETN the most.

This section has presented information that is based on theoretical considerations. It is important to note that the amount of CO recovered from calorimetry tests of high explosives (secondary explosives) is reported to be far larger than the amount predicted by equilibrium calculations. A study by Ree et al. (1995) points to the effect of cooling on the detonation equilibrium, thus slowing the reaction.



Ree et al. (1995) report that the computed moles of CO in the detonation products from a mole of PETN, using the theoretical Chapman-Jouguet (C-J) point, is 0.126 moles, but based on the slowed reaction, the resulting CO value is 1.63 moles. The C-J point is based on the theory that says the detonation point is a state in thermodynamic and chemical equilibrium and is independent of pressure and temperature. If one can deduce that field results are more closely related to calorimetric test findings than theoretical estimates, then there is the real possibility that models will underestimate CO generation.

2.1.2 Modeling of CO Generation

Scientists at the Lawrence Livermore National Laboratory, Energetics Materials Center, have developed computer models that use basic thermochemistry to predict detonation products and physical conditions for a wide variety of explosives. Their most recent model, CHEETAH, contains information on many explosives, including those used in oil well perforation. The model allows the user to select explosives of interest and conditions under which the explosives are detonated. These conditions include open (default), gun, and confined space detonations, all of which were used in RTI's model runs. In addition, there is an option to run the model where CO₂ is excluded from the detonation products, which is both a worse case situation and possibly representative of conditions at some perforating zones in wellbores.

Model results, in general, for perforating explosives varied modestly for most combinations of conditions and energetic material (explosive). The explosives modeled were HMX, RDX, HNS, PYX, and PETN. RDX and PETN have become the most commonly used explosives in modern drilling techniques, including deviated or horizontal wellbores. Thus, they were modeled under the largest number of conditions.

CHEETAH finds the equilibrium in reactions at specified pressures and temperatures. The detonation standard run is based on C-J detonation theory and is a one-dimensional detonation. The

transformation of explosive to gaseous products is assumed to be very fast at steady state. The standard run calculates the C-J state, then models the expansion of the product gases to one atmosphere or until a standard temperature is reached (298 EK). Typically, this takes place over approximately 10 microseconds. Although the program can calculate thermodynamic states where temperature and pressure are not explicitly indicated, the default results reflect a simple characteristic of the chemical reactions—detonation products are those predicted by complete combustion, and the chemical equilibrium between CO₂ and CO is estimated, keeping the total moles of each element fixed (C, O, etc.). Results are independent of the amount of explosive used, so one can scale the model outputs proportionally to any amount of explosive.

For purposes of this task, RTI estimated total grams of CO generated for each combination of explosive and condition, based on the following assumptions:

- # 4-inch high-explosive guns (HEGs)
- # 80 grams of explosive used per foot of perforation zone
- # 250 feet of perforation.

This translates into a total of 20 kg of explosive.

Individual CHEETAH model outputs are provided in Appendix A. Table 2-2 shows CO estimates generated using 20 kg of explosive. The two scenarios, one including and one excluding CO₂ from the detonation product mix, were run for each explosive. Table 2-2 includes the amount of CO generated in grams, moles of CO per kg of explosive used, and percentage of CO in the total detonation product volume.

There are similarities in detonation physical characteristics among the explosive used in oil well perforations (e.g., detonation pressures and detonation velocities). The amount of CO predicted is only slightly more variable, on the order of 2-fold differences between explosives. Under CHEETAH's standard detonation, CO is a significant fraction of the detonation gases when all carbon is oxidized to CO and no CO₂ is generated, ranging from 13% of total gases from HMX to around 60% for HNS and PYX.

Conclusions drawn from the CHEETAH modeling include

- # The volumes of CO generated are a significant fraction of the total detonation gases even with CO₂.
- # The estimated volume of CO ranges from approximately 0.1 m³/kg of explosive to 0.5 m³/kg explosive. These volumes of gas would be significant if released in confined spaces.
- # The estimates of CO generated are more closely tied to the amount of explosive and type of explosive than whether detonated in a gun, in a confined space, or in the open.

Table 2-2. CHEETAH Carbon Monoxide Results for Perforating Explosives

Explosive	Scenario 1: Explosion with CO ₂ accounting							Scenario 2: Explosion excluding CO ₂				Increase in CO, % (from Scenario 1 to 2)	Conditions
	CO, mol/kg explos.	CO, % vol	CO, g	CO, vol, m ³	CO ₂ , mol/k g explos.	CO ₂ , % vol	CO ₂ , g	CO, mol/k g explos	CO, % vol	CO, g	CO vol, m ³		
HMX	4.7	13	2,636	2.3	4.8	13	4,224	13.48	33	7,549	6.6	186	Standard Detonation
RDX	10.9	27	6,093	5.3	2.607	5	2,294	13.49	33	7,554	6.6	24	Gun
RDX	10.9	27	6,093	5.3	2.607	5	2,294	13.46	33	7,538	6.6	201	Gun. Confined Space
RDX	6.0	16	3349	2.9	4.475	12	3,938	13.5	33	7,560	6.6	126	Standard Detonation
RDX	6.0	15	3349	2.9	4.475	12	3,938	13.47	33	7,543	6.6	125	St Detonation, Conf Space
HNS	10.7	37	6,003	5.2	5.207	18	4,582	19.95	60	11,172	9.8	86	St Detonation
PYX	9.0	30	5,023	4.4	5.87	20	5,166	20.09	58	11,250	9.8	124	St Detonation
PETN	6.8	19	3,752	3.3	9.486	27	8,348	15.80	40	8,848	7.7	136	Gun
PETN	6.8	19	3,752	3.3	9.486	27	8,348	15.80	40	8,848	7.7	136	Gun, Confined Space
PETN	5.9	17	3,304	2.9	9.884	29	8,698	15.79	40	8,848	7.7	168	Standard Detonation
PETN	5.9	17	3,304	2.9	9.884	28	8,698	15.79	40	8,848	7.7	168	St Detonation, Conf Space

Assumes: 80 g explosives/ft for 4" HEGs

250 ft of perforation = 20 kg explosive

24.5 L/mol of gas; Mol. wt. CO₂ = 44 g/mol, Mol. wt. CO = 28 g/mol

CO estimates from the CHEETAH model were used in conjunction with simple engineering assumptions to estimate release rates at a well head. The concentration of CO in ambient air near the release point were estimated using two EPA dispersion models, the OCD5 offshore model and ISC-Prime, an onshore model.

2.1.3 Ambient Modeling of CO

Two ambient dispersion models were used to estimate ambient concentrations of CO.

- # Offshore Model. The *Offshore and Coastal Dispersion*, model version 5, (OCD5) was used to simulate the effects of offshore emissions from a point source located on platform. The OCD5 model was developed by Earth Tech, Inc., for the Minerals Management Service, and the model was taken from the EPA's web site SCRAM (Support Center for Regulatory Air Models) (EPA 2000). The OCD5 model includes special algorithms that account for overwater plume transport and dispersion, as well as changes that take place as the plume crosses the shoreline. In addition, the OCD model also includes treatments of plume dispersion over complex terrain and platform downwash.
- # Onshore Model. The EPA's refined dispersion model, *ISC-PRIME*, was used to estimate the air concentration from an onshore release. The ISC-PRIME model is also available on EPA's web site (EPA 2000). The new building downwash algorithms were incorporated into the latest version of the Industrial Source Complex Short Term Model (ISCST3), and the revised test bed model was named ISC-PRIME.

Both models calculate the hourly air concentrations for each receptor and outputs only the maximum hourly air concentration at each receptor location. Meteorological data were gathered for coastal California, one set for onshore (from Oakland station) and one set for offshore (near Santa Barbara). The single most important portion of information for modeling is wind speed. Lowest annual one hour wind speeds for each 10 ° of direction are a primary determinant of the maximum hourly concentrations, in this case, of detonation gases.

Assumptions about release speed and release angle were made in order to model ambient concentrations of CO. The assumptions for the modeled scenarios were based, in part, on volumes of CO from the estimated by the CHEETAH program and also included the following:

- # vertical and horizontal releases
- # a release speed of 3 meters per second
- # a release height of 5 feet
- # a point release

- # releases of CHEETAH-modeled CO occur over a period ranging from 5 minutes to one hour.

The results of the modeling are presented in terms of concentration (ppm) per CO release rate in grams/second (g/s).

The Gaussian plume model is the basis of both ambient concentration models. This means that the concentration of a pollutant, in this case CO, at a distance from a source is a function of wind speed and the lateral and vertical dilution factors. The ambient concentrations estimated by the models are directly proportional to the release rate. Table 2-3 summarizes the results of the two models. Note that the values presented in the table are based on wind speeds which were the highest annual average hourly concentrations for all 36 receptor directions (360 E divided into 10 E-increments). “Average concentration” is the arithmetic mean of the 36 receptors and maximum concentrations are the highest 1 hour values at 5 meters.

Appendix B provides the full complement of hourly unit concentrations for each of the receptor directions for the representative onshore and offshore locations. In Table 2-3, offshore locations were assumed to have no building interference in air flow, while the onshore location is assumed to have a building interference. Buildings have a significant impact on air flow, causing both turbulence (greater mixing within a zone of influence) and pockets of less mixed air. The estimates presented should only be considered as qualitative estimates of worst-case unit concentrations. They allow the risk assessor to estimate whether CO concentrations could be in a range that could cause acute effects for those individuals in the area.

The results from the CHEETAH program combined with the unit concentrations from the ambient models allow one to estimate potential exposure levels. These exposure estimates are presented in Table 2-4. The data suggest several things.

- # Dilution of CO over the distances modeled are significant due to Gaussian principles, where wind and increasing plume cross-sections greatly reduce the CO concentrations.
- # Point releases of CO on the order of 2 to 10 m³, even over a 5-minute period, are diluted significantly with natural air flows.

2.2 Engineering Review

Basic features of an oil well and perforation are discussed in this section. It is provided to support the understanding of borehole perforation, what types and volumes of explosives are used, and what physical factors may influence the amount of CO generated from well perforation.

Table 2-3. Estimated Onshore and Offshore Unit Concentrations of Carbon Monoxide^a

Location, discharge direction	Distance from Release, meters	Avg CO Concentration (Standard Deviation) ppm per g/s release	Maximum CO Concentration ppm per g/s release
Offshore,			
vertical discharge	5	4.2 (0.01)	4.2
	10	9.8 (0.01)	9.8
	20	6.5 (0.06)	6.6
	30	5.1 (0.2)	5.5
horizontal discharge			
	5	16.7 (0.58)	18.5
	10	14.4 (0.23)	15.1
	20	7.9 (0.14)	8.2
	30	5.7 (0.18)	6.0
Onshore			
vertical discharge	5	8.0 (0.9)	9.8
	10	7.0 (0.9)	8.7
	20	8.1 (2.1)	12.1
	30	6.7 (3.7)	13.6
	40	4.1 (1.4)	7.2
horizontal discharge			
	5	19.4 (2.9)	27.7
	10	15.4 (3.4)	20.8
	20	12.8 (3.3)	23.5
	30	8.4 (4.0)	15.5
	40	5.2 (1.9)	8.5

^a Offshore Model = OCD5, Onshore Model = ISC-Prime; Unit Concentration is ppm of CO per gram/second release.

Table 2-4. Estimated Ambient Concentrations of Carbon Monoxide ^a

Explosive	Detonation Condition	CO Generated ^b , kg per 20 kg of explosive	CO concentration in Detonation Gas, ppm	Estimated Ambient Concentration ^c , ppm			
				Offshore		Onshore	
				vert rel	horiz rel	vert rel	horiz rel
HMX	standard	7.55	330,000	104	176	201	489
RDX	gun	7.55	330,000	105	176	201	490
	gun, confined space	7.54	“	104	175	200	490
	standard	7.56	“	105	176	200	490
	standard, confined space	7.54	“	104	175	201	490
HNS	standard	11.2	600,000	155	260	297	724
PYX	standard	11.2	580,000	156	262	299	729
PETN	gun	8.8	400,000	122	206	235	573
	gun, confined space	8.8	“	122	206	235	573
	standard	8.8	“	122	206	235	573
	standard, confined space	8.8	“	122	206	235	573

^a CO ambient concentrations are based on total CO generated released in 5 minutes. Gaussian plume models predict the ambient concentrations.

^b CO generated are the values from CHEETAH with CO₂ excluded from the detonation products (maximizing CO generated); these values may not represent the worst-case conditions, because calorimetry tests have shown higher CO generation rates than predicted by theorems. 1 kg of CO is equal to 0.8732 m³ at standard pressure and temperature.

^c Ambient concentrations are those estimated for 5 meters from the release point. Concentrations at points farther can be scaled based on values presented in Table 2-3.

2.2.1 Operational Considerations

The following discussion focuses on the drill rigs and perforation. The site where exposures to CO may take place is the well head, which contains valves, flanges, seals and flow lines that may be sources of CO release. Figure 2-1 presents a generic wellhead.

2.2.1.1 The Drill Site and Drill Rigs.

Onshore. At land sites where the operator has contracted for the drilling of a deep, high-pressure well, a work crew may dig a rectangular pit, or cellar. The cellar is usually lined with concrete or wood; it provides additional working space to accommodate the installation of drilling equipment beneath the rig floor. A tall stack of high-pressure control valves is located in the cellar. The typical cellar size is about 10 feet on a side and, perhaps, 10 feet deep. The exact size and depth depend on the characteristics of the well and the configuration of the rig.

For land rigs, a substructure raises the rig floor (the work area for the drilling crew) anywhere from about 10 feet to 40 feet above the ground. With the rig floor elevated above ground level, room is available under the rig for the high-pressure valves and other equipment that the crew connects to the top of the well's casing.

The land rig will also have a derrick or mast. A derrick is load-bearing structure erected over a well site to provide support for drilling equipment and is used to raise and lower drill pipe and casing. A mast is a simple portable derrick, consisting of a sturdy A-frame used for drilling shallow wells, or for workovers of damaged wells, and is held upright by guy wires. If the rig has a mast, crew members raise it from horizontal to vertical with draw works. (Sometimes, this is called a jackknife derrick rig.) If the rig has a derrick, usually called a standard derrick, crew members bolt it to the substructure.

Offshore. Offshore rigs perform the same function as land rigs; however, their design is more complex. The types of offshore drilling rigs include the barge, jackup, fixed platform, semi-submersible, drill ship, and other, newer, deep-water types of drilling rigs. A schematic of various types of offshore drill rigs is found in Figure 2-2.

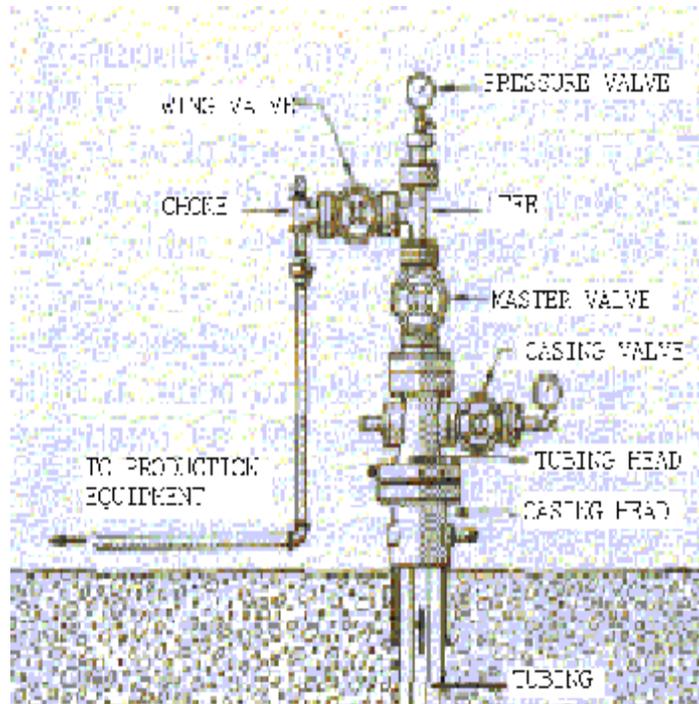


Figure 2-1. Wellhead.

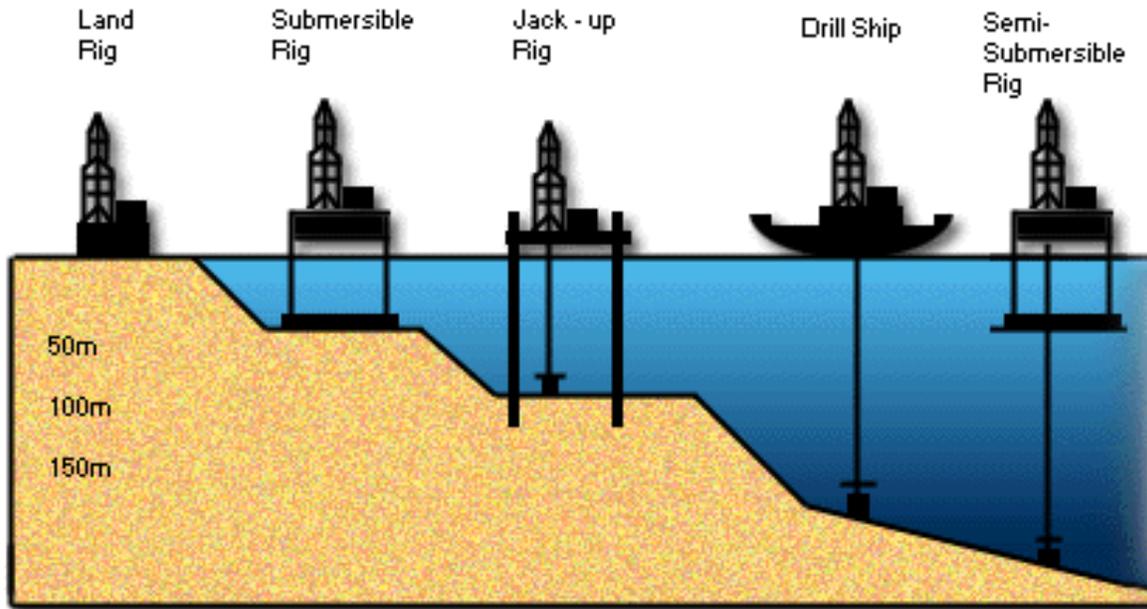


Figure 2-2. Types of drilling rigs.

A barge is used in shallow waters or in swamps up to 50 feet deep. It is a shallow-draft, flat-bottomed vessel equipped with a jackknife derrick.

A jackup rig operates in water as deep as 350 feet and is very stable because it rests on the sea floor. The jacket of the jackup rig is slowly towed to its location during calm seas, then the legs are lowered with jacks until they rest on the sea floor below the deck. The legs continue to lower until the deck is level and lifted off the surface of the water, sometimes clearing 60 feet. Jackup rigs can be moved from location to location.

The fixed-platform operates in water up to 1,350 feet and is secured to the sea floor with long steel pilings. They are very stable and are considered permanent and virtually immobile.

Semi-submersible rigs can also operate in water as deep as 8,800 feet. They are stable but are not fixed. These rectangular floating rigs carry a number of vertical stabilizing columns and support a deck fitted with a derrick and related equipment.

The drill ship offers the greatest mobility. It is specially constructed or converted for deepwater drilling, and can operate in almost any water depth. Dynamic positioning equipment (computer-controlled propellers along the hull that continually correct the ship's drift) keeps the ship above the wellbore using a thruster with controllable pitch propellers.

The main function of the rig is to make a wellbore (also called a borehole or hole). To make the hole, the drilling crew place a bit on the sea floor, then the drill rotates the bit and pumps drilling mud into it. The rig components include power, hoisting, rotating, and circulating systems.

The power system transfers power with either a mechanical or electrical transmission. Electric rigs are easier to maintain than mechanical rigs; they do not require chains and sprockets to transfer power. Both mechanical and electrical rigs need a hoisting system.

The hoisting system consists of the draw works, the derrick, the crown block, the traveling block, and wire rope drilling line.

The rotating system includes devices that turn the bit. For a conversion rig, the equipment consists of the swivel, a special length pipe called the kelly, an upper kelly, the upper kelly cock, a lower kelly cock, a kelly saver sub, the rotary table, the drill pipe, the drill collars, and the bit.

Drilling fluid and circulation equipment form the circulation system. The equipment includes the components of the rotating system, the mud pump, the discharge line, the stand pipe, the annulus, the return line, the shale shaker, the desilter, the desander, the mud pits, and the section line.

2.2.2 Well Completion – Well Perforation

Well completion is the process of preparing a newly drilled well for production. Perforation is the piercing of the casing wall and cement to provide holes through which formation fluids may flow. It is accomplished by lowering into the well a perforating gun that fires electrically detonated bullets or shaped charges. In general, well completions are categorized as casing completions, open-hole completions, and drainhole completions. The most common, casing completions, are used 90% of the time. They can be further subdivided into five subcategories

- # conventional perforated casing completions,
- # permanent well completions,
- # multiple-zone completions,
- # sand-exclusion completions, and
- # water- and gas-exclusion completions.

After an oil or gas well is completed, the wellbore is isolated from the surrounding geologic formation using casing and cement. With conventional perforating casing completions, the casing is cemented through the production interval and communication (movement of material) between the formation and wellbore is established with perforation. Adequate communication between the wellbore and all desired zones within the wellbore, as well as isolation between zones, is essential to evaluate and to optimize production and recovery from each zone. Establishing fluid communication between the wellbore and formation, for either production or injection, requires some perforating operation. A cross-sectional view of the basic elements of a wellbore is found in Figure 2-3.

2.2.2.1 Overview of Perforating Methods. Several different systems, including bullet perforating, high-pressure water jets or sand laden slurries, and jet perforating, are used to create perforations in wellbores.

Bullet Perforation. Bullet perforation is among the oldest perforation methods. The original bullet perforator was created and patented in 1926. With the bullet-perforating method, propellant-driven bullets are shot through casing and cement into the formation. A steel carrier, called a gun, conveys the bullet penetrators downhole. The penetrator is fired by sending an electrical signal down a wireline to ignite the propellant. The burning propellant accelerates a bullet through a short barrel (2 inches or shorter) at velocities (up to 3,300 feet per second) sufficient for the bullet to penetrate casing, cement sheath, and formation. However, bullet-penetration performance decreases substantially in high-strength formations and when very high-strength casing is used. Currently, bullet perforators are used infrequently for specialty applications, such as soft formations, brittle formations, or where consistently round holes in casing are needed.

High-pressure Water Jets or Sand-Laden Slurries. Another perforating method uses high-pressure water jets or sand-laden slurries to abrade a hole into the casing, cement, and formation. With the high-pressure water jet method, a tool that uses a pump to force high-pressure fluid through a flexible, extending lance is conveyed downhole, and the lance jets its way into the formation, creating very clean tunnels with little or no formation damage. The major disadvantage, however, is that the process is slow and expensive, and the holes must be created one at a time. Thus, the process is impractical for long intervals. In the case of sand-laden slurries, the slurry is pumped down the tubing and turned at the bottom by a deflector and nozzle arrangement that allows the fluid stream to impinge directly on the casing. Holes and slots are made, and the casing can even be cut completely by manipulating the tubing.

Jet Perforation. Jet perforating, the most widely used perforating technique, involves the use of high explosives and metal-lined shaped charges. Jet perforators are conveyed in a wellbore using several methods, including slickline, electric line, coil tubing, and production tubing.

Jet penetration from a shaped charge occurs with a jet pushing material aside radially, which results in formation of a hole. Material in the formation is not removed; however, it is displaced. The process of forming a jet stream involves a chain reaction comprised of different explosive components.

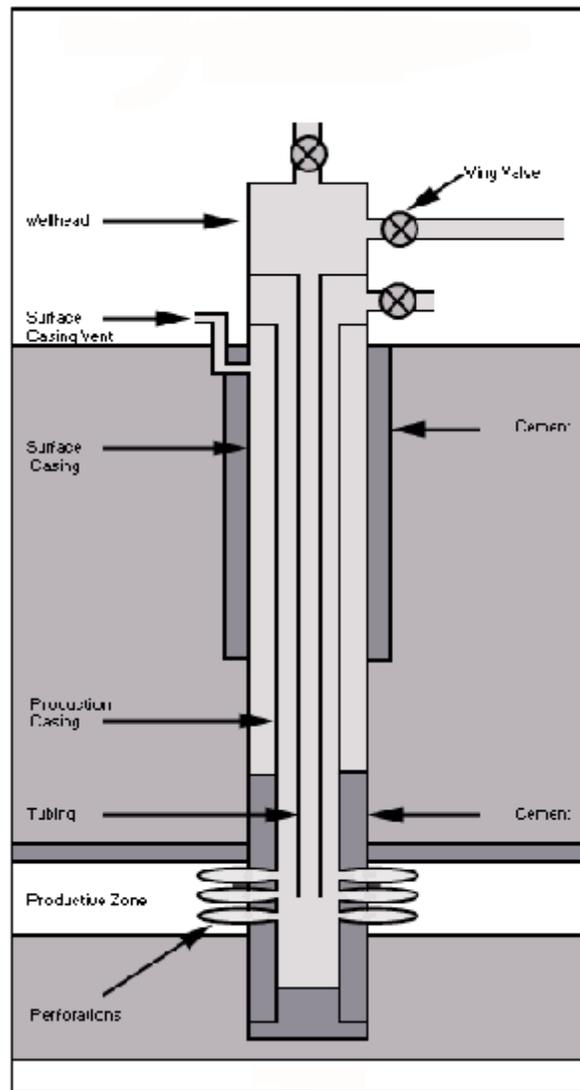


Figure 2-3. Simplified cross section of a well bore.

The chain reaction, or explosive train, begins with a detonator, or initiator. It successively detonates the detonating cord (which transmits a detonation along the longitudinal axis of the gun), the high-velocity booster in the charge, and finally, the main shaped-charge explosive. The shaped-charge explosive perforates the casing and penetrates the cement sheath and formation.

High explosives. The high explosives used in these components react supersonically when initiated with the detonation process. (Low explosives react subsonically in a process called deflagration and are generally not used in jet-perforating applications. Examples of low explosives are propellants and gunpowders; TNT is an example of a high explosive.) The explosive generates a high pressure that causes the metal in the charge liner to flow. A continuous pressure buildup on the liner causes a needle-like, high-speed jet of fine particles to spew from the cone at a speed of about 20,000 feet per second at its tip, with a pressure estimated to be 10 million pounds per square inch (psi). This stream of liner particles is the key to the perforating process. The target is pierced by the focused force stream, leaving rubble and a compressed zone immediately adjacent to the perforation.

High explosives can be subdivided into primary and secondary explosives. The sole purpose of primary explosives is to start the detonation reaction with a small energy input, which is usually accomplished by heating an electrical filament wire or by impact. Lead azide and lead styphnate are two examples of primary explosives. They are sensitive to energy inputs from heat, flame, friction, impact, and static discharge. Because of their sensitive nature, primary explosives must be used with great care (Economides et al., 1988).

Secondary high explosives are used in three component of the explosive train: detonators, detonating cords, and shaped charges. These explosives are much less sensitive to external stimuli than primary explosives; therefore, they are safer to handle. However, due to their insensitivity, they can be difficult to initiate, but once initiated, secondary explosives release tremendous amounts of chemical energy in microseconds. For oilfield use, the most widely used secondary explosives are RDX, HMX, HNS, and PYX (Economides et al., 1988). More recently, the perforating guns have also used PETN as a high explosive. A summary of the explosives and relevant properties is provided in Table 2-5.

Perforations are performed under pressure differentials between the wellbore and the pressure in the geologic formation. Two types of perforating conditions are underbalanced perforating and overbalanced perforating.

Underbalanced perforating. Underbalanced perforating occurs when the pressure in the wellbore is lower than the pressure in the formation. When used properly, this technique can effectively provide higher productivity completion. Underbalanced perforating creates an environment where formation fluid flow can begin to enter the wellbore immediately, rather than having the well in an overbalance condition where completion fluids and other particles continue to be lost into the formation. At the instant of perforation, the pressure differential to the wellbore is believed to help clear the perforations and remove crushed rock, debris, and explosive gases from the formation. Formation fluid type and reservoir permeability are the two primary factors influencing the amount of underbalance level to remove a portion of the crushed rock and other damage mechanisms from the near-wellbore area (Economides et al., 1988).

Table 2-5. Secondary Explosives Used in Perforation

Common Name	Chemical Name	Relevant Properties				
		Chemical Formula	Oxygen Balance, % by wt	Heat of Formation, ?H/kJ kg ⁻¹	VOD ^a , ft/sec	DP ^b , psi
PETN	Pentaerythritol tetranitrate	C ₅ H ₈ N ₄ O ₁₂	-10.13	-1703	27,200	NA
RDX	Cyclotrimethylenetrinitramine	C ₃ H ₆ N ₆ O ₆	-21.60	+279	28,700	5,000,000
HMX	Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine	C ₄ H ₈ N ₈ O ₈	-21.62	+253	30,000	5,700,000
HNS	Hexanitrostilbene	C ₁₄ H ₆ N ₆ O ₁₂	-42	+128	24,300	3,500,000
PYX	2,6-Pyridinediamine, 3,5-dinitro-N,N'-bis(2,4,6-trinitrophenyl)-	C ₁₇ H ₇ N ₁₁ O ₁₆	-53	NA	24,900	3,700,000

^a velocity of detonation

^b detonation pressure, psi

Sources: Economides et al., 1998 and Akhavan, 1998

Studies (King et al., 1986; Behrmann and McDonald, 1995; Crawford, 1989) have suggested that the instantaneous underbalance must be followed with continued, sustained flow of several gallons per perforation to further clean the perforation, and to remove the crushed rock and other materials that have been loosened. This point is critical and well documented, yet it is often overlooked on many jobs. A large influx of hydrocarbons into the well is undesirable because it will increase the complexity of any other well activities that are planned.

Underbalanced perforating is operationally much easier with tubing-conveyed perforating systems or if a single wireline perforating run is possible. Proper underbalance levels and continued flow are often not effectively used on wireline operations where multiple gun runs are required. Achieving appropriate underbalance levels with other intervals contributing flow and back pressure is operationally difficult. Some operators are concerned about continued wellflow after perforating because debris can possibly be produced above the perforating guns and wireline being retrieved from the wellbore (Economides et al., 1988).

Numerous technical articles have been written to compare the underbalanced perforating technique with overbalanced perforating both in the laboratory and in field studies (Economides et al., 1998).

Overbalanced perforating. In many low-permeability formations, remaining reservoir pressures are insufficient to effectively clean the perforations (as suggested by King et al., 1985 and others). In

other instances, formation competence is questionable, and the risk of sticking the perforating guns with high underbalance levels makes the use of underbalanced perforating methods an operational risk. Extremely overbalanced perforating is a near-wellbore stimulation technique used in conjunction with the perforating event. The method has gained popularity within the past few years because of the large number of wells that could not be effectively perforated using underbalance techniques. Extreme overbalance perforating also provides perforation breakdowns in preparation of other stimulation methods and, thus, eliminates the need for conventional breakdown methods (e.g., breakdowns of perforation in carbonate formation) (Economides et al., 1988).

During extreme overbalanced perforating jobs, most of the tubing is pressurized to high overbalance levels with compressible gases, which have high levels of stored energy, above relatively small volumes of liquids. Upon expansion at the instant of detonation, the gases are used to fracture the formation and to divert fluids to all intervals. The high flow rate through relatively narrow fractures in the formation is believed to enhance near-well conductivity. Field data also suggest that high initial pressures are more likely to create fractures within the perforated interval and to limit height growth.

Recently, perforating systems have been developed to release propping material downhole with the gun detonation so that the extremely overbalanced fluids and nitrogen rushing to the formation carry erosive and propping materials. Currently, most of the extremely overbalanced perforating jobs are designed with pressure levels set a minimum of 1.4 psi per foot of true vertical depth. The technique is also being used to obtain a production test in very low-permeability formations before more large, expensive stimulations. While most jobs are conducted using tubing-conveyed perforating systems, some completions with short intervals have used wireline perforating methods (Economides et al., 1988).

2.2.3 Thermal Decomposition of Explosives – Safety Factors

Time-temperature curves have been experimentally generated for various explosives. Figure 2-4 depicts a set of curves for HNS, HMX, PYX, and RDX. The curves provide guidelines about the probability of quiet decomposition versus violent events. As long as a particular explosive stays below its time-temperature curve, it will function properly—quiet decomposition.

The curves are applicable for conditions where explosives are exposed solely to the effect of temperature. For gun system conditions, where the explosive components are exposed to both temperature and pressure, the time-temperature relationship is different. As an example, HMX detonating cord is normally rated at 400 EF for one hour at ambient temperature and pressure, as shown in Figure 2-2, but laboratory tests show it can undergo violent reaction after only 8 minutes when subjected to the simultaneous conditions of 400 EF and 15,000 psi. Thus, pressure serves to accelerate the decomposition reaction.

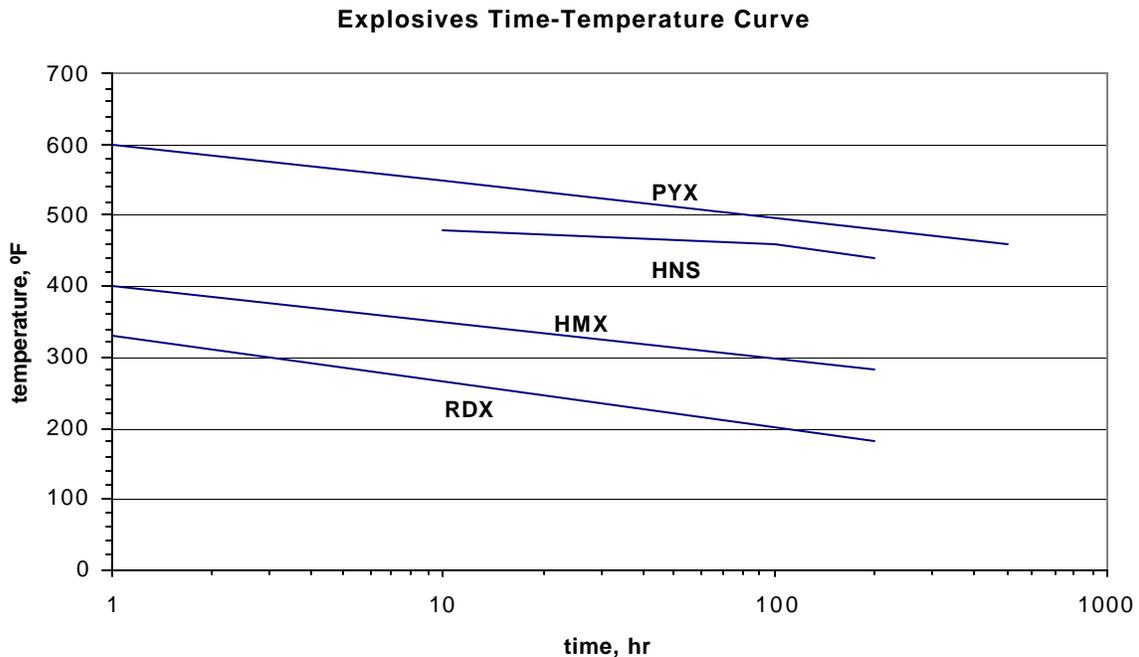


Figure 2-4. Time-temperature curve for perforating explosives

(Schlumberger 2000 and Economides, 1998)

2.2.4 Perforating Gun Systems

Gun perforating systems are designed to satisfy several perforating criteria. They continue to evolve in response to the need for more efficient and complete production of petroleum from wells and a growing dependence on production from deeper, more remote, or more challenging geological formations. What is presented here is only a summary of gun system basics with brief discussion of those elements as they may relate to higher amounts of explosives and, therefore, CO production.

Gun systems involve a physical carrier system that delivers a detonating chord, an electrical circuit, and a shaped charge (carrying the working explosive) in a configuration designed to deliver penetration depth and hole sizes that satisfy the flow of materials in and out of geologic formations. The whole system is considered as the perforating gun or perforating tool. A number of elements make up the system(Allen and Roberts, 1993)

- # **A detonator**, sometimes called a blasting cap, is made up of a primary explosive and is very sensitive to shock and temperature. The detonator initiates the firing sequence, which can be initiated through a firing pin, pressure increases, or by electrical signals.
- # **A detonating chord** carries the high-order shock wave to detonate each shaped charge.

- # **A shaped charge (perforator)** is made up of a case, a primer charge, the main explosive such as PETN or RDX), and cone shaped liner. Shaped charges are arranged in a variety of ways, depending on the number of charges desired, the carrier system, and the nature of the geologic formation (see Figure 2-5).
- # **A penetration mechanism**, which is a jet stream by which metallic particles are thrust into the target. Penetration depth and hole size are functions of liner strength, charge weight and liner shape.

Shaped charges have been developed with increasing size (diameter) to increase the size of the opening through the casing and into the formation. The range of gun sizes are from less than 2 inches to over 7 inches. Casing hardness and wall thickness also affect penetration characteristics. The amount of explosive used with each charge is proportional to the size of the charge. Table 2-6 presents representative explosive loadings associated with charge size. Along with the number of charges per foot, one can determine the amount of explosive used, which, in turn, is directly related to the amount of CO generated. The generation of CO is discussed Section 2.3.

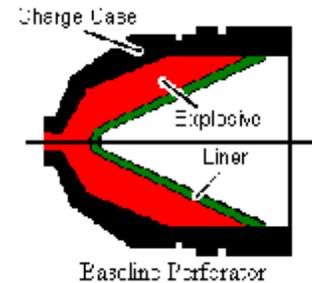


Figure 2-5. Perforator cross-section.

(<http://www.owenstools.com/API/Hydrocode/default.htm>)

The carrier systems (carrying the shaped charge, detonator chord and detonator) have changed along with the size, shape, and types of explosives used in the charge. They can be broadly grouped as **through-tubing gun, casing gun, and end-of-tubing gun.**

The expendable through-tubing perforator carries smaller charges and may leave more debris in the hole than other types. Its main advantage is that it is easily adapted to underbalanced perforating in short zones. No shutting of the well to pull the gun or manipulate the tubing is needed, and it usually results in higher productivity. The smaller, thinner-walled carriers carry smaller guns, such as a 1 and 11/16-inch or 2 and 1/8-inch guns.

An example of the through tubing perforator is shown in Figure 2-6 (Schlumberger, 2000).

Casing guns are conveyed by wireline and are associated with two types of carriers, a reusable port-plug or a counterbored non-reusable type. Both are retrievable and leave no debris, casing damage is minimal and, in the case of port-plug guns, they can be used up to 100 times. Port plugs are used under less demanding conditions, such as in wells with moderate hydrostatic pressures and temperatures. Wireline-conveyed guns are more limited in the amount of weight that can be put down a well. Longer perforation intervals require multiple gun runs and, following an initial run, underbalance perforation may not be as effective because formation fluid inflow normally reduces the underbalance. Another type of perforator associated with the wireline-conveyors is the capsule perforating gun, where charges are encapsulated, and since there is no thick walled carrier involved, they can be larger than the hollow tube guns. A major disadvantage, however, is the detonator and detonator chord exposure to wellbore fluids.

Table 2-6. Representative Amounts of Explosive for Perforating Guns

Gun Size, inches	Casing Size, inches	Gun Type	Avg. Explosive Load, g
1-11/16	4.5	Capsule	10.5
2-1/8	5.5	Capsule	15
3-1/8	4.5	Port Plug	11.5
4	5.5	Port Plug	21.1
5	7	Port Plug	32
1-9/16	4.5	Scalloped	3
2	4.5	Scalloped	6.75
2-7/8	4.5	Scalloped	12.5
3-3/8	4.5 or 5	Scalloped	22.7
4-5/8	7	Scalloped	25
5	7	Scalloped	30
7	9.625	Scalloped	56.5

Source: Halliburton, 1998. API RP-43 5th edition. Data Summary, 8/21/98.

The end-of-tube gun is run on the end of the tubing, and the charges can be detonated mechanically by dropping a metal bar down the tubing..

Tubing-conveyed perforators were developed to extend underbalanced perforating to long sections in deviated holes offshore. Either retrievable reusable (port plug) or retrievable non-reusable (scalloped) configurations are used and charge types, shot density, and phasing are similar to wireline-conveyed casing guns. Scalloped guns (counterbored) are used in the most demanding well conditions and are the mainstay of tubing-conveyed perforating operations.

2.3 Case Studies

A limited number of reports are available that address issues of particular relevance to the risk of exposure to CO at an oil well. The reports discussed below build the case that CO is a real risk factor when explosives are used.

The first two reports are oil industry specific, one being the Seacliff oil well accident (Vintage Petroleum) and the second involving monitoring for CO during oil well perforation (Goodman Well). Following these two reports, we present case studies which show similar CO exposures from explosive use (Section 2.3.3) and also present reports from EPA that summarize monitoring data from the detonation of explosives (2.4).

2.3.1 Vintage Petroleum Incident - August 10, 1994, Ventura County, California

2.3.1.1 Introduction. The Vintage Petroleum incident involved the death of three workers who were overcome by CO. In 1995, the families of the deceased workers sued the oil company. Among several court depositions, one by Mr. Toby Thrower, head well-puller with Pride Petroleum, provided a number of details involved in the accident. The following discussion is based on his deposition.

2.3.1.2 Background. Pride Petroleum was contracted by lessee, Vintage Petroleum, to a well (Well C-10A of the Vintage Petroleum Hobson Lease, operated under CDOGGR permit No. P923-482), to convert the idle producer to a wastewater disposal well. The well had previously been completed in the Pliocene Pico formation above and below the Rincon fault (upper deep and deep zones 8635–11,630 ft) and was being recompleted into the Pliocene Pico formation (shallow zones 2120–2815 ft).

Schlumberger Wireline Service was contracted to conduct well perforation for the conversion. A Mr. Crawford was a consultant hired to direct the perforation. Mr. Thrower of Pride Petroleum had converted producing wells into water disposal wells on the same lease more than 15 times.

2.3.1.3 Key Daily Activities. On August 2nd, 1994, upon arrival at the site, Mr. Thrower described the well as having a riser on it and coming out of an 8 ft x 8 ft x 9 ft cellar with wooden cellar boards on top. The riser came off the top of the flange, and the flange was bolted to the 7-inch casing. A flow line came off it that went to a trap about a quarter mile away from the well. The trap was in use when the well was producing. A 16-inch casing was down lower in the cellar.

Pride's crew had to remove the flange and installed a 6–9-inch blow-out preventer (BOP) to the well-head. The BOP is a valve designed to stop the release of pressure. (The BOP played a role in the

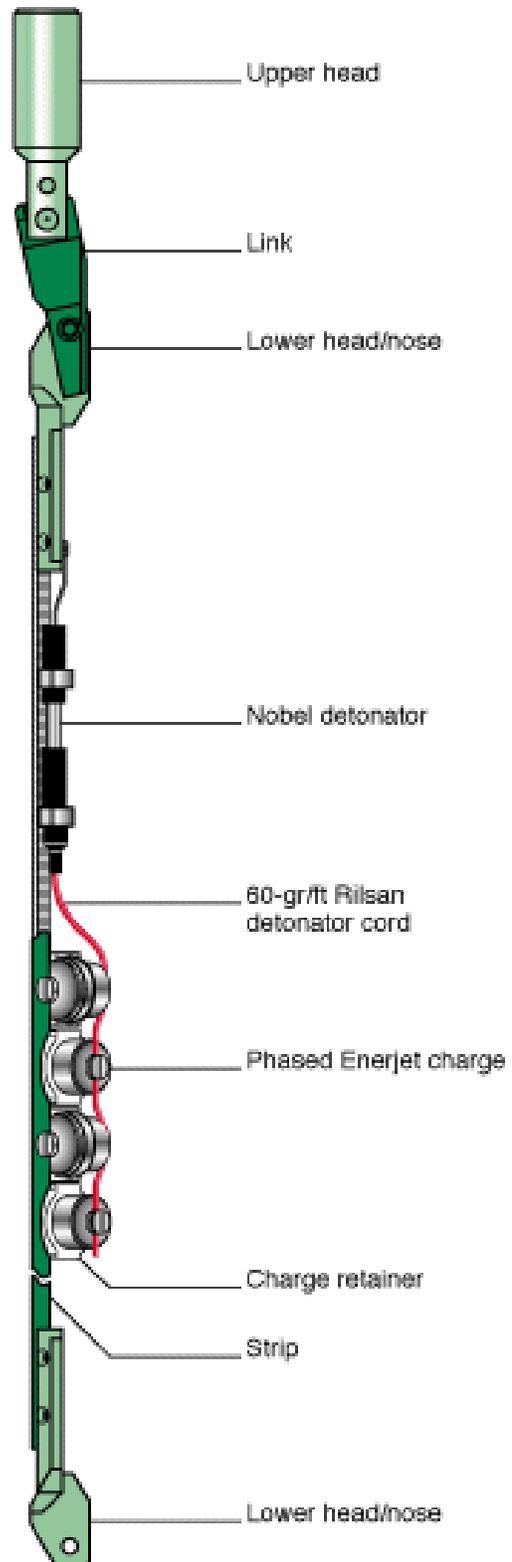


Figure 2-6. Through-tubing expendable gun system.

accident as described later in this summary.) The BOP remained open to pull a pipe through and lower it into the well casing. The riser and the BOP were in the middle of the cellar. Two inches of the BOP was above the cellar boards; most was below the plane of the cellar.

They removed the flow line from the well head and installed two 1500 psi working pressure valves.

On August 3rd, the Pride crew rigged up the pump to the well head, and bled the casing and the tubing down. They pumped 32 barrels (bbls) of clean, filtered water down the casing with the returns from tubing to the vacuum truck. They recovered about 20 bbls of oil. They switched the line to the pump pit and continued circulating the well clean for 20 minutes, after which, it lay dead.

On August 4th, the Pride crew opened the well and observed a release of pressure on the casing and tubing. They removed the circulating head and installed a shooting flange and a “packoff” for Schlumberger. NOTE: On prior conversions, the perforator company had a lubricator, not a packoff, but Mr. Thrower did not think it odd because, from the available information, the well was thought to be in a “thief zone.” This is a zone that will take water. In such a zone, there is just hydrostatic pressure or very little pressure. In a thief zone, a lubricator would not be needed, because one would not expect to encounter gas.

They rigged up the wire line truck, ran electromagnetic casing log from 4500 ft to the surface, and ran the NL-CCL log from 4500 ft to 1500 ft. They rigged out the wire line truck and filled the casing with clean, filtered water. Later, they poured silica 30 sand down the casing, which, mixing with lease water, closed the well. The sand lies on top of the bridge plug so that if a bit is run back to clean out, the sand is seen first before the bit reaches the bridge plug.

On August 5th, upon reopening the well, they had a slight blow (puff of air [composition unknown]) in the casing from some pressure buildup, then they ran in the hole with the perforating gun. At 3,981 feet, they shot four ½-inch holes in the 7-inch casing. They rigged the wire line truck, and they filled the 7-inch casing and pressured to 1800 psi because they established that they were taking fluid. This pressured the water out through the perforations. No returns or blow occurred afterwards.

Pride also performed a “squeeze job” intended for zone isolation so there would be no more leakage in that zone

On August 6th, Pride rigged the Schlumberger and shot four ½-inch holes at 1510 ft. They got a blow at the Baker tank from the 16-inch casing, so they plugged it with a Halliburton EZ drill SV packer. They filled the space between the 7-inch casing and the 16-inch casing.

August 7th was not addressed in deposition.

On August 8th, the Pride crew pressure tested the 7-inch casing to make sure there were no leaks.

On August 9th, no records were provided, but the deposition states that the crew finished drilling out the EZ drill plug. One worker went into the cellar to install a 16-inch valve. Because there were open perforations in the well, and because the cellar was considered a confined space, the worker was harnessed. They tested for gas before entry with a Bendix tester for H₂S. The meter did not measure other gases.

On August 10th - the day of the incident, Schlumberger arrived and installed the shooting flange, rigged up the wire line into the derrick, and prepared to perforate. Pride held its daily 5-minute safety meeting and then a safety meeting with Schlumberger. The focus of the second meeting was on the distance the Pride crew maintained while Schlumberger ran their equipment in and out of the well. Pride did not have any type of respiratory equipment as this was not considered a “gassy well.” Pride never encountered H₂S or methane in the Hobson lease wells.

Schlumberger began to run in the perforating guns. During that time, the Pride crew changed a valve out on the back of the circulating pump that was leaking. They also pulled the heads on the pump and cleaned the cement and checked underneath.

Perforation occurred over 352 ft at 4 perforation shots per ft, creating 1,408 perforation holes. At 11 a.m., Mr. Thrower noticed water coming to the surface during the perforation interval from 2,138 to 2,815 ft. A 20-ft expended perforating gun was being withdrawn from the well when the flow started. The water was 6–8 inches above the metal grating on the cellar boards and was shooting out of the 7-inch casing valve (i.e., the 2-inch pipe that was screwed into the 7-inch casing. A valve, which could be hooked up on a flow line to the mud pit, was located about 6–8 inches out from the casing. A steel line had been hooked up and connected to the mud pump previously; however, it was disconnected (per consultant Crawford’s direction) while Pride was disconnecting the circulating head on the morning of the 10th. This was so Mr. Crawford could monitor the well for any flow that would come out of the 2-inch pipe, while the crew was perforating. (Any flow coming out of the 2-inch pipe indicates fluid or gas coming into the casing from the shoot hole’s zone.) Mr. Thrower testified that they do not normally disconnect the steel line. Crawford chose to monitor from the well, not the pit, because he was sitting in his car from which he could view the well better.

Mr. Thrower notified Mr. Crawford of the leak. Mr. Crawford said that “the well was a thief,” because they were perforating in a thief zone. Mr. Thrower testified that he believed he could monitor a well as easily at the mud pit hooked to the steel line as at the well head cellar.

After Mr. Thrower notified Mr. Crawford, the perforation process continued, and water continued to rise a little higher after a few runs. Mr. Crawford said not to worry because he had several guns left to shoot and that he might get lucky and catch a thief zone.

After three or four more guns were run, the fluid started coming up probably 10 or 12 ft. Mr. Crawford said it would be best to close the well, and the Pride crew proceeded toward the well to close the water in (i.e., close the 7-inch valve). To do so, they had to remove some of the floor grating and contain the water flow to get a crescent wrench onto the valve itself and shut it.

The crewmen could not reach down inside the valve. They had a 5-gallon bucket held by two crewmen's hands over the hole from which water was flowing over the 2-inch pipe, directing the fluid into the cellar. Because of the bucket and two crewmen, there was no room to get to the valve, so they removed a couple of cellar boards to try to reach the valve and close it. Water was blowing up like a fountain, and they couldn't see to work.

When they still couldn't reach the valve, one worker, Jason, stood on the BOP with his foot on the 7-inch flange on the bottom of the BOP and his other foot on about the 2nd rung of the cellar. He then leaned over the cellar, and he said he still could not reach the valve. Jason, standing upright on the BOP with one foot over on the wall, threw a crescent wrench up on the cellar. Mr. Thrower picked up the wrench and walked out between the pipe rack and threw the wrench on the ground.

When Mr. Thrower returned a few seconds later, he did not see Jason standing anywhere. He looked down in the cellar and Jason was unconscious in the cellar. Water in the cellar was 3–3 ½ ft deep. Subsequently, two other men entered to rescue Jason, but both were overcome and died also.

2.3.1.4 Potentially Important Facts About the Incident.

- # On August 9th, the crew only tested for the presence of H₂S, which proved negative.
- # The Pride crew had never encountered H₂S on methane in the Hobson lease wells.
- # On August 10th - the day of the accident - no respirators were on-site
- # A steel line had been hooked up and connected to the mud pit previously. However, it was disconnected (as per consultant Crawford's direction) while Pride was disconnecting the circulating head on the morning of the 10th.
- # The choice was made to use a packoff seal, rather than the lubricator seal traditionally used.
- # The decision to monitor the well, not the mud pit, for water flow was apparently made for convenience.
- # The decision was made not to cease perforation upon discovery of flowing water.
- # 1408 holes were shot in 352-ft zone on August 10th.
- # The crew attempted to reduce or cap the uncontrolled flow of water by physically placing a bucket of solvent on top of the rig leak.
- # Access to the 7-inch valve that would have stopped the unexpected flow of water was poorly accessible.

- # The crewman attempting to close the 7-inch valve was not harnessed.
- # The crewman attempting to close the valve was not standing in a safe position—one foot was on the BOP and one foot was on a ladder rung in the cellar.

There were a number of decisions made about the crew's physical actions (e.g., lack of harnessing, improper stance, no respirators, etc.). These occupational safety decisions contributed to the incident; however, RTI believes these decisions fall outside the scope of this study. The number of holes shot, the lack of monitoring for gases, the disconnection of the line from the well to the mud pit, the proximity of crew fatally exposed to the leak, and the level of worker exposure all relate to the generation and transport of CO. RTI addresses these factors in Section 4.1, Safety Procedures.

2.3.2 Summary of Perforation Monitoring at Goodman 1 - June 27 - July 1, 1995

2.3.2.1 Introduction. Following the Vintage Petroleum accident, the State of California was interested in examining the potential for significant CO levels related to perforation exercises at oil wells and to the court case involving Vintage Petroleum. The information summarized here is based on two sources, a deposition of Mr. William J. Wright, Production Foreman, Seneca Resources; and a memorandum from Bill Wright, Seneca Resources, to Barry McMahan, Well Files, and California Division of Oil, Gas, and Geothermal Resources, September 20, 1995.

2.3.2.2 Background. Seneca was contracted to clean the well out to its total depth, perforate some more holes in the casing, run a packer above the perforations, and convert it to a water injection well. Schlumberger was contracted to perform the perforations with HEGs in the area of the hole that was previously a production area (i.e., the injection zone was going to be the same as the prior production zone).

2.3.2.3 Key Daily Activities. On June 24th, 1995, Mr. Wright acquired CO testing equipment, a Passport brand quad meter supplied by Secorp, for the site. The quad meter reads four functions: lower explosive limit, oxygen, H₂S, and CO. The quad meters were believed to be self-calibrating and had warning indicators on battery levels. He also acquired air packs (30-minute escape packs).

On June 27th, Mr. Wright did not install a vent line. Rather, he ordered a lubricator with a pack-off at the top of the pipe. It was Seneca policy always to use a lubricator. A full lubricator covers the length of the gun so if pressure were encountered, one could pull the gun up into the lubricator and close the BOP and, in turn, secure the well. A partial lubricator (i.e., a packoff with the short lubricator) will not allow the crew to close the BOP. Gas monitoring occurred at the end of a blowdown line (a hose 35–40 ft long) that was attached to the 2-inch casing valve that came off the 5½-inch casing (full casing depth was 5½ inches). The blowdown line was run downwind in a southwest direction. Mr. Wright stated that the casing valve was open to the blowdown line during the perforation process even though, in this case, there was no concern about unsafe pressure buildup during the detonations.

Schlumberger Wireline Service arrived onsite. Mr. Wright arranged for Schlumberger to monitor fluid levels in the wellbore during the perforation process (indicated by weight change of HEG). Fluid level was observed by Mr. Wright (who was in the Schlumberger cab) during each of the runs. Mr. Wright stated that he documented the fluid level before the perforation began but was still trying to locate the records (the “tour reports”). He testified that during perforation, the fluid level was rising.

Mr. Wright stated that this well was overbalanced, meaning that if the wellbore filled with water, that water would push back into the formation. He added that there was no known H₂S-type risk with the well. The American Petroleum Institute (API) reading on the oil was “fairly light,” meaning not tarry or heavy crude.

Mr. Wright recalled that a safety meeting was held with the Seneca crew to discuss CO risks. He explained to the crew that Schlumberger was using the same type of shooting system used at Rincon. He also explained where the crew could and could not stand at all times (i.e., they were restricted from the discharge of the blowdown line).

Perforation, using 11 HEGs in series, occurred over about 5½ hours. During perforation, no liquid was discharged from the blowdown line. Mr. Wright did not use protective equipment to monitor the gas exiting the blowdown line. Instead, he approached the line’s end from upwind and held the monitor by the strap to lower it to the end of the blowdown line. Mr. Wright knew that the Permissible Exposure Limit (PEL) established by the Occupational Safety and Health Administration (OSHA) was 35 parts per million (ppm). Mr. Wright measured for CO before perforation began (0 ppm reading); he testified that he measured for CO after firing each of the 11 guns. He further stated that he did not measure CO during the perforation. However, he did measure CO right after they shot the last (11th) HEG. The alarm triggered, and the meter read 855 ppm. The crew pulled the gun up into the lubricator. The well’s BOP was shut and secured, and the casing valve was closed.

On June 28th, a Secorp safety technician arrived on-site, donned a 30-minute air pack, went to the well, opened the casing valve, went to the end of the blowdown line with a Passport quad meter, and measured for gas. He reported verbally to Mr. Wright that he immediately read the meter’s maximum reading of 900 ppm. The Secorp representative then secured the well and closed the casing valve.

On June 29th, another Secorp representative arrived with a Draeger tube (a colorimetric CO measuring device) manufactured by Sensidyne, that is capable of measuring higher levels of CO. The tube measured 20,000 ppm at about 11 a.m. when the casing valve was first partially opened. At the same time, 50 psi of pressure was bled off over about a 5-minute period. The second measurement was 200,000 ppm (20%) without using a plastic sampling bag. The third measurement, 10–15 minutes later, using a bag sampler, was 500,000 ppm (50%). After the third CO test, the crew pumped 180 bbls of lease water in the well using a “hot oil” truck to knock down the gas into the formation.

On June 30th, a Secorp representative again tested for CO in the early morning, using the same Draeger tubes, but Mr. Wright was uncertain if Secorp used sampling bags. Secorp measured 300,000 ppm (30%) CO. Mr. Wright’s crew then pumped 120 bbls of lease water into the well.

During the last 25 bbls pumped, they saw pressure build up indicating the well was filled. As soon as the hot oil truck shut down, the well became overbalanced, and the fluid level began dropping, indicating to Mr. Wright that they had not encountered a pressure barrier. None of the crew tried to determine whether a gas bubble existed that expanded, causing the fluid level to rise during the pumping. Throughout the 5 hours of water pumping during the morning, no CO was detected during frequent testing. After the 5 hours, the crew began measuring a really light flow of CO at 5,000 ppm.

Mr. Wright contacted Schlumberger's Bakersfield office that day. He said he was "making a courtesy call so Schlumberger could warn [his] people and [his] customers that indeed...there is CO involved in perforating" (Wright 1995).

On July 1st, CO measured again at 400,000 ppm (40 %).

This was the final day of activity reported. It appears the well was closed indefinitely.

2.3.2.4 Potentially Important Facts About the Incident. The crew prepared for the job by acquiring a CO meter and air packs.

- # The quad meter was brought on-site was inadequate to measure the higher levels of CO.
- # The crew installed a full lubricator to capture retrieved HEGs safely.
- # The crew set up a blowdown line placed to emit gas downwind of well of the crew.
- # The blowdown line exit gas was monitored for CO.
- # Mr. Wright monitored the fluid level during perforation.
- # No history of H₂S was known for the well.
- # The well was known to be overbalanced.
- # A safety meeting on CO risk and restrictions on crew location was held before perforation began.
- # Eleven HEGs were used in series over the course of 5½ hours.
- # CO readings were taken.

June 27	855 ppm	quad meter measured by Seneca
June 28	900 ppm	quad meter maximum measured by Secorp
June 29	20,000 ppm	partially open valve, measured with Sensedyne Draeger tube
June 29	200,000 ppm	no sampling bag; open air measurement

June 29	500,000 ppm	measurement of bag sample
June 30	300,000 ppm	measurement of bag sample
June 30	5,000 ppm	measurement after pumping 120 bbls of lease water
July 1	400,000 ppm	(use of sampling bag unknown)

- # Upon the first reading—855 ppm on quad meter—the crew chief wisely decided to close the well and seek a more accurate CO measurement.
- # On July 29th, 50 psi of pressure was measured upon opening the valve.
- # During high CO measurements, 5 hours of water pumping into the well suppressed the CO to 0–5,000 ppm
- # The well was closed upon determination that a high CO level was sustained following recovery from last water pumping.

In this incident, the awareness of CO emission potential and the corresponding preparatory measures taken by Seneca resulted in safer incident management. However, the levels of CO eventually measured demonstrated the need to have more accurate monitoring equipment on-site at the beginning of the job. As with the Vintage incident, a large number of holes were shot over a short period of time using the same product—HEGs—and, coincidentally or not, CO was emitted at lethal levels had the workers been exposed. This reinforces the need to determine any correlation between the HEG explosive material (PETN), the number of shots over time, and the potentiometric conditions of the deposit (over- or underbalanced), among other factors. These are addressed in the following sections of this report.

2.3.3 Harvest Platform, Chevron, Santa Barbara County, California

On February 2, 1998, there was a release of gas on Chevron's offshore Platform Harvest. Chevron issued a Near Miss/Incident Report. As stated in the report, "...CO had not been a problem on other perf jobs because of the short intervals being shot. However, this well had over 4800 shots fired, creating a larger volume of gases being generated. No winds were blowing to dissipate CO as it came to the surface. Only required gas monitors being used are H₂S & LEL..."

The company had anticipated the potential for gas releases at the platform by providing hand-held monitors and assuring that breathing devices were available and in working order. At an earlier meeting, the staff discussed safety issues, including preparation for possible toxic gas exposures. A hand-held monitor was used to measure CO levels that had a top measurement limit of 500 ppm. This level was reached and the actual ambient concentrations are not known.

Following this accident, MMS issued a Safety Alert advising operators to take reasonable precautions to protect personnel when long intervals are being perforated. As stated in the Safety Alert, MMS Pacific OCS Region recommends, as a minimum, that (1) CO monitoring equipment, large

capacity fans, and supplied air breathing units be made available and maintained operational during all extensive perforating operations, and (2) this subject be covered during pre-operations safety meetings, which should be attended by contractors. Later in 1998 additional CO testing was reported in a performance record for the Harvest Platform. H₂S, explosive limits (LEL), and CO measurement values are provided. CO was reported at 50 ppm.

2.3.4 Non-oil Field Incidents of Explosives Use and CO Poisoning

In the peer-reviewed literature, there were several additional reports of accidents where people were potentially exposed to CO from explosives used near the surface and below-ground. The construction and mining industries are important users of explosives; some of the same explosives used in oil well perforation.

There are both important differences and similarities between the petroleum, construction, and mining industries that specifically relate to the potential for CO exposures. It appears that CO poisoning, though well known from internal combustion engines, has only recently been described for these other industries.

A few summary remarks are provided at the end of this section, following the summaries of three published reports.

2.3.4.1 Construction Site Explosives Contaminate Home, Quebec City, Canada.

Auger et al. (1999) report of CO poisoning in a dwelling where “probable source of contamination was the use of explosives at a nearby rain sewer construction site.” Two adults had to be treated for CO exposure, and the investigators tested the home and neighboring houses for CO.

CO was measured through ventilation pipes that were installed under the foundation of the home of the exposed individuals with an initial reading of 500 ppm. The source of CO was very likely the use of explosives at a nearby construction site. Samples from the trench where the explosives were used gave concentrations up to 700 ppm. Two explosive products had been used in the construction site excavation

- # a mixture of ammonium nitrate, sodium nitrate, and fuel oil (Apex Ultra 40; ICI Canada, Inc., North York, Ontario, Canada); and
- # a mixture of ethylene dinitrate and glycol/nitroglycerine (POWER FRAC; ICI Canada, Inc.).

Both sets of explosives have a negative oxygen balance and form CO. The reported CO generation rates for these explosives (in lab) are

- # Apex Ultra 40 - 15.9 L of CO/kg
- # POWER FRAC - 22.3 L of CO/kg.

The authors also suggest that because the blasting was performed underneath a layer of soil, there was an oxygen deficiency. This likely produced increased amounts of CO over that tested in the laboratory. Another factor may involve the rock where blasting occurred. It was a “limestone high in carbonates which, with intense heat, may generate CO.” Measurements at the house continued, and contamination lasted one week

In a second incident reported by Auger et al. (1999), six houses in a neighborhood in a small town in Quebec were also contaminated with CO following nearby rock-blasting for sewage system connections. Six of 16 occupants were intoxicated with CO. After levels subsided, blasting resumed.

The specific explosives were not specified, but the reported CO readings in the homes were

- # Round 1, Day 1 - in-house readings ranged from 125 to 600 ppm
- # Round 1, Day 2 - in-house readings negative
- # Round 2, Day 1 - in-house readings negative in 5 of 6 houses
 - S nearby manhole reading as high as 1,100 ppm
 - S Round 2, Day 2 - in-house reading in 6th house = 52 ppm.

Installation of ventilation shafts was required to eliminate all residual CO from the 6th house.

2.3.4.2 Manhole Contaminated from Explosives. Deitchman et al. (1998) report another case of CO poisoning due to explosives use in construction. Employees worked in a “newly installed, unconnected manhole, finishing shortly before underground explosives were detonated 50 ft south of the manhole to break up rock and soil. A worker entering the manhole 45 minutes after the explosion collapsed within minutes, as did two coworkers who rescued him. One worker died.”

Nitroglycerine-based explosives were placed 18 ft deep in 2½-in diameter drilled holes with 265 pounds of explosive distributed in 22 boreholes and detonated.

- # The CO generation rate of explosive reported from laboratory testing was 27 liters of CO per kilogram (kg).
- # Readings of CO in the manhole were reported as
 - S Day 1 - 600 ppm at 6 ft depth
 - S Day 2 after incident
 - near 0 ppm at the surface of manhole
 - over 1,000 ppm (monitoring device limit) at the bottom of manhole
 - 1,910 ppm (after manhole was filled with groundwater and then pumped until nearly dry) at 11-ft depth
 - 40 ppm at 7-ft depth.

The authors speculated as to factors that contributed to CO exposure. They stated that fractures in the rock created by the explosion and the soil structure contributed to pathways of movement for the CO to the manhole.

2.3.4.3 Detonation of Explosives in a Testing Tunnel. Velsko et al. (1999) in a report to the *Fifth Conference on Life Cycles of Energetic Materials* (Orlando), provided evidence of the formation of CO and the efficiency by which the explosives are converted to complete combustion products. Conventional munitions and rocket motors were subject to contained, full-scale detonation (of projectiles) and burning (of rock motors) in the NTS X-Tunnel to characterize emissions. The X-Tunnel is a 600-ft-long mined area, and the leaktight test chamber's dimensions were 100 ft long, 50 ft wide, and 35 ft high (total volume about 164,000 cubic feet [ft³]).

Material detonated was M107, 155-mm high-explosive projectiles. The process resulted in conversion of C4, Composition B, and supplemental charge explosives to several products.

- # C4 = 91 % (wt) RDX, 5.3% di(2-ethylhexyl)sebacate, 2.1% polyisobutylene, 1.6% motor oil
- # Composition B = 63 % (wt) RDX, 36% TNT, 1% wax
- # Supplemental charge = 98.5% TNT, 1.5% barium stearate.

They did not report quantitative CO generation rates, but did state, "Gaseous products of explosive or propellant reactions are chiefly nitrogen, CO, and water (H₂O). The atmosphere in the chamber provided the oxygen to convert the CO to carbon dioxide." However, for munitions, the CO₂ concentration was determined to be slightly lower than expected. CO and other products of incomplete combustion were also present. Overall conversion of the explosive carbon to gaseous products ranged from 85% to 94%. The conversion to CO₂ appeared to max out in the chamber during the first 500 seconds of monitoring following detonation.

2.3.4.4 Summary. Modern explosives are used in a variety of industries, including the petroleum, construction, mining, and space/rocket industries. The conditions under which the explosives are used vary considerably and, therefore, the potential for CO exposure may be quite different. In the petroleum industry, there is a nearly closed system that gives the well operators the ability to control the potential releases of CO. The situation at any above-ground construction site, for example, is far different from that at a wellhead. CO may be generated over a wide area and dissipated based on the ambient conditions and location of structures or other barriers. Mining operations may be above- or belowground, and even belowground, explosions may take place over a much wider area than found at a petroleum site.

In all cases, there are safety measures required; a central safety element is having informed foremen and workers who understand the potential for CO generation and exposure, among the other hazards. Despite the rarity of CO poisoning due to explosives in any of these industries, CO is a known byproduct of explosives use. These case studies show what CO levels may be generated and what the consequences may be in situations where CO is unanticipated.

2.4 Monitoring Data Collected

The single most important report of CO monitoring at an oil well undergoing perforation is that described in Section 2.3.2. Monitoring performed by the State of California at the Goodman well during late June 1995 presents the most direct evidence of CO in the wellbore from perforation, measuring CO up to 500,000 ppm from the casing valve.

Three studies are described in this section, all dealing with detonation gases for a range of explosives.

2.4.1 Mitchell and Suggs (1998)

Mitchell and Suggs (1998) developed emission factors for explosives when detonation occurs by open burning or open detonation. The study was performed by the EPA using data collected by the U.S. Department of Energy.

Twenty-three energetic materials (both high and low explosives in bulk and assembled [encapsulated]) were detonated in a 930-cubic-meter (m^3) chamber called a BangBox located at Dugway Proving Ground. One set of experiments was conducted in a standard atmospheric environment of the BangBox. The second experiment used bags of water to suppress the detonations for two, TNT-based materials with diverse oxygen contents—amatol (mixture of ammonium nitrate and TNT) and tritonal (2-methyl-1,3,5-trinitrobenzene with aluminum). The suppressed experiment was designed to represent the effect on emissions of detonation under a soil cover.

The explosives were made up of the following components: TNT, RDX, Tetryl, PETN, Al KNO_3 , NA, NC, and NG. Their findings included:

- # For unconfined detonations, the median percentage of recovery of carbon as carbon oxides ($CO_2 + CO$) was 98.5%; only 1.6% of the carbon was recovered as CO.
- # Detonating an energetic under a soil cover (buried detonation) will cause a decrease in CO_2 and an increase in soot, CO, light saturated hydrocarbons (and certain organics).
- # The composition of the initial detonation products is not greatly affected by the degree of confinement, but the composition of the final products is affected. *The more oxygen-deficient the energetic, the more the degree of confinement affects the final product mix.*
- # The products formed by detonating an energetic in an inert atmosphere (e.g., CO_2) will be essentially the same as those formed when the energetic is detonated in a vacuum.
- # The distribution of carbon in emission products from detonating TNT in different atmospheres in a bomb calorimeter were

- %C as CO in a vacuum = 28% of the calorimeter's atmosphere;
- %C as CO in O₂ atm = 5%; and
- ratio of 5.6:1.

2.4.2 Ornellas (1974)

A study by Ornellas (1974) concluded that the actual composition of initial detonation products depends on a variety of factors; one of the most important is the amount and form of oxygen in the energetic molecule. If the energetic is oxygen-balanced or only slightly oxygen-deficient, most of the carbon is converted to CO₂. As the oxygen-balance becomes more negative, the amount of soot, CO, and other incompletely oxidized products formed increases and the fireball must occur if the incompletely oxidized products formed by the detonation are to be converted to CO₂, nitrogen gas (N₂), and H₂O.

2.4.3 Mitchell and Suggs (1998)

Mitchell and Suggs (1998) summarizes detonation results from seven studies. This research included PETN found in the following items detonated: FMU-149, FMU-54, ARD-446, BBU-36, MK-107, Det train, M43A2, M-158, M-206, Det cord, and GCU-2A. The emission factors in the validated database are calculated based on the total mass detonated, rather than those which result when the actual mass of PETN and RDX is used. Mitchell and Suggs compared the original emission factor for percentage of CO of CO_x to the adjusted emission factor, which resulted when the actual mass of PETN is used to calculate the emission factors.

Emission Factors for PETN (kg of CO per kg of C in explosive)

	<u>Original</u>	<u>Adjusted to Actual PETN</u>
Median	1.45E-05	2.55E-04
Mean	1.28E-04	6.74E-04
Std. Dev.	2.33E-04	8.78E-04
# of explosives tested	10	10

In his comparison of emission factors derived from water-suppressed detonations of amatol (oxygen balanced) and tritonal (severely oxygen deficient) to those derived from the unsuppressed detonations of these materials, Mitchell and Suggs (1998) showed that, consistent with Ornellas' research, *quenching the afterburn significantly increases the emissions of incompletely-oxidized species ... and sharply decreases the emissions of CO₂*. He noted placing an oxygen source in contact with the explosive molecules will not ensure an efficient detonation when it is conducted under a soil or water blanket cover. In his comparison of CO emission factors for unsuppressed and water-suppressed detonations of tritonal and amatol, he found

Emission Factors for Tritonal and Amatol, Unsuppressed & Water-Suppressed Detonations

Emission Factors			
Explosive	Water Suppressed	Unsuppressed	Ratio of Suppressed to Unsuppressed
Tritonal	27E-02	29E-04	93
Amatol	2.3E-04	9.7E-04	0.24

These results dramatically shows the effect quenching has on an oxygen-deficient explosive.

The environment underground in an oil or gas well is one in which water or other fluids are present. Despite the Mitchell, Suggs, and Ornellas untested factors of high temperature and pressures as found in perforation zones, it is reasonable to assume that combustion of carbon in perforating explosives is incomplete, even for the inherent oxygen in the explosive's molecule.

3.0 Hazard Identification - Acute Toxicity of CO

CO is a very well known toxic gas that is a major concern in many industries and for public health. A review of the health effects of CO are provided in this section. Information is also provided on the relationship between exposure concentrations of CO, the level of carboxyhemoglobin in the blood, and the health consequences.

3.1 Introduction

CO is a colorless, odorless, tasteless, and nonirritating gas formed as a by-product of burning organic compounds. It is also a leading cause of poisoning deaths and morbidity in the United States, with about 10,000 cases reported each year (Benaissa et al., 1999; Marius-Nunez, 1990). Fires are the leading cause of CO exposures and deaths. Other sources include stoves, furnaces, portable heaters, automobile exhaust, charcoal grills, and tobacco smoke. Poisonings are often associated with improperly ventilated heating systems, malfunctioning or blocked exhaust systems, and suicide attempts. In addition, exposure to methylene chloride, a volatile solvent used in paint thinners and degreasers, can result in CO poisoning because it is metabolized to CO in the liver.

3.2 Absorption and Elimination

CO is rapidly absorbed by the lungs and most of it rapidly binds to hemoglobin, forming carboxyhemoglobin (COHb). The hemoglobin binding affinity of CO is 230–270 times greater than the binding affinity of oxygen; therefore, low air concentrations of CO can be dangerous. About 15% of absorbed CO binds to myoglobin and blood proteins. Elimination is through the lungs with a half-life of about 3–4 hours. Breathing 100% oxygen reduces the half-life to 30–40 minutes, and breathing hyperbaric oxygen at 2.5 atmospheres reduces the half-life to 15–20 minutes; therefore, oxygen and hyperbaric oxygen are used to treat CO victims (Ellenhorn and Barceloux, 1988).

3.3 Acute Toxicity

CO exposure impairs oxygen delivery and utilization by reducing the oxygen-carrying capacity of the blood, reducing oxygen release by increasing oxygen binding to hemoglobin, and inhibiting cellular respiration (Thom and Keim, 1989; Miró et al., 1998, 1999; Ellenhorn and Barceloux, 1988). Low barometric pressure, high lung diffusion capacity, high alveolar ventilation rate, high metabolic rate, and reduced cardiac output increase CO toxicity. The fetus, young children, the elderly, and individuals with cardiovascular disease are at the greatest risk from CO poisoning.

Exposure to high concentrations of CO can be rapidly fatal due to hypoxia and cardiac dysrhythmias. Symptoms of lower exposures include headache, nausea, chest pain, confusion, diarrhea, fatigue, blurred vision, shortness of breath, dizziness, weakness, fainting, and seizures. Although CO can affect many organs and systems in the body, those with the highest oxygen requirement (e.g., heart and brain) are particularly susceptible. Acute poisonings commonly result in brain damage, persistent neurologic dysfunction, and cardiovascular injury. Even after recovery from CO poisoning, delayed neurologic symptoms occur in about 10% or more of the victims. These delayed effects occur within 1–4 weeks following exposure and may include amnesia, hallucinations, urinary incontinence, disorientation, apathy, aphasia, personality changes, and seizures (Ellenhorn and Barceloux, 1988; Thom and Keim, 1989).

Other organs and systems that may be affected include the skin, lungs, blood, muscles, and kidneys. Skin bullae, alopecia, and sweat gland necrosis are relatively rare, and cherry red skin is very rarely seen in survivors of CO poisoning. Pulmonary edema, aspiration pneumonia, hemolytic anemia, thrombocytopenia, rhabdomyolysis, and acute renal failure may occur in severe cases (Ellenhorn and Barceloux, 1988).

Although clinical effects may vary substantially with COHb levels, Table 3-1 provides a general correlation of COHb levels and symptoms. However, age and health status of the victim and the pattern of exposure are important factors regarding mortality and morbidity. For example, seizures and coma have been reported at COHb levels of 30–40% in cases where exposure exceeded 12 hours (Lacey, 1981). Furthermore, COHb levels alone do not completely explain CO toxicity. Impairment of cellular respiration through inhibition of cytochrome c oxidase may be responsible for many of the persistent effects following acute CO poisoning (Miró et al., 1998, 1999; Wilson et al., 1998). CO concentrations as low as 100 ppm or 0.01% in air can cause clinical effects within 2 hours. At 200 ppm CO, COHb levels can reach 30% (Ellenhorn and Barceloux, 1988). The current occupational threshold limit value (TLV) recommended by the American Conference of Governmental Industrial Hygienists (ACGIH) for a 40-hour work week is 25 ppm.

3.4 Diagnosis and Treatment

CO poisoning is not easy to recognize because the signs and symptoms are nonspecific and mimic many common conditions (e.g., headache, seizures, nausea, fatigue, flu-like symptoms, unstable angina, unconsciousness) (Balzan et al., 1996). If CO exposure is expected, treatment with 100% oxygen should begin immediately, and COHb levels should be measured. Although somewhat controversial, treatment with hyperbaric oxygen is indicated for (1) unconsciousness or seizing, (2) cardiac arrhythmia or ischemia, or (3) COHb levels greater than 25% (even with minor symptoms) or greater than 20% for children or pregnant women (Balzan et al., 1996). There is some evidence that hyperbaric oxygen therapy administered as late as one month following exposure may alleviate some neuropsychiatric symptoms (Coric et al., 1998). However, there can be complications with hyperbaric oxygen therapy. These include rupture of the tympanic membranes, pulmonary edema, decompression sickness, pneumothorax, damaged sinuses, and cerebral gas embolism (Balzan et al., 1996; Ellenhorn and Barceloux, 1988).

Table 3-1. CO Poisoning and Symptoms

CO in atmosphere, ppm	COHb Concentration (%)	Symptoms
<70	< 10	No appreciable effect
70 - 120	10–20	Possible headache with throbbing temples, shortness of breath with moderate exercise
120 - 220	20–30	Headache, irritable, easily fatigued, possible dizziness, dim vision
220 - 520	30–50	Severe headache, dyspnea at rest, nausea, abdominal pain, weakness, confusion, blurred vision, fainting on exertion, ataxia, increased heart rate
520 - 1,200	50–70	Unconsciousness, seizures, bradycardia, depressed respiration, coma
>1,200	>70	Respiratory failure, death

Sources: Lacey, 1981 and Ellenhorn and Barceloux, 1988.

4.0 Review of Relevant Regulations and Industry Procedures and Guidelines

4.1 Safety Procedures

Explosives are inherently dangerous. For the oil industry, rules of explosive safety are generally followed and there is a good safety record. In addition to physical safety concerns, health hazards exist at a well site. This report focuses on the potential exposure to CO whose risks can be managed in standard industry ways. The single most important element in managing CO risk is knowledge that well perforation generates CO in significant amounts.

Human error frequently causes industrial accidents. The Seacliff well accident is an unfortunate example where poor human judgement was the single most important cause of fatalities. Standard oil industry safety practices of proper venting, use of personal protective equipment, and providing support to individuals entering a dangerous space were all violated.

Safety procedures for working in potentially toxic environments, particularly those with immediate acute risks, already exist in the oil industry. H₂S is an extremely hazardous gas associated with oil and gas wells. Proper respect for its toxicity is found in the safety procedures developed by the industry and governmental agencies. These same plans and actions are applicable to CO and other noxious gases that may exist or be generated in an oil wellbore.

Knowledge that CO is generated during oil well perforation reinforces the need to maintain worker and management safety training. Armed with the understanding that CO could be released requires a steady vigilance as to workplace hazards. No longer can those involved believe that if H₂S is absent from a petroleum well, there is little to fear from wellbore releases.

Pressure control equipment is required when perforating is taking place with underbalanced conditions or when there is any possibility that the well may flow after perforating. A system that includes blowout preventer, hydraulic tool trap, lubricator risers, head catcher and check valve, grease injector pump, and hydraulic packing nut assembly is needed for maintaining control of well pressures. Maintaining pressures with such systems rated from 5,000 to 15,000 psi are needed.

Safety procedures for well perforation need be reiterated and reinforced to include

- # CO monitoring;
- # venting of cutoff and other valves away from sites of human activity;

- # maintaining control of well pressures to reduce venting of fluids and gases from the bore, and
- # worker training, provision of respirators, and first aid.

This list merely outlines the general areas of safety that will reduce the potential for CO and, therefore, the risks associated with perforation.

A representative set of safe work practices was developed by an oil company involved in onshore and offshore drilling. Their safe work practices can be summarized as

- # no venting of fluids and gases to the drill deck;
- # train personnel in monitor use and maintenance, confined space work practices, emergency response, personal protective devices, and lines of communication and responsibility;
- # monitor for CO continuously on the drill floor and at venting points using appropriate, dedicated, and maintained instruments;
- # provide positive ventilation in confined spaces; and
- # handle spent perforation guns properly.

4.2 CO Regulations and Guidelines

There were no specific regulations identified for CO exposure from the use of explosives either at the federal or state level. An advisory developed by the State of California for reducing the potential of CO exposure at offshore platforms was the only industry-specific action that could be found.

Table 4.1 summarizes more generic federal and state regulations and guidelines involving health and safety for CO.

Table 4-1. Regulations and Guidelines for CO

Agency	Description	Information	Reference
<u>NATIONAL</u>			
Environmental Protection Agency (EPA)	National Ambient Air Quality Standard	9 ppm (10 mg/m ³) - 8-hr avg 35 ppm (40 mg/m ³) - 1-hr avg	40 CFR 50.9
Occupational Safety and Health Administration (OSHA)	<i>Permissible Exposure Limit (PEL)</i>	50 ppm (50 mg/m ³)	29 CFR 1910.1000, Table Z-1-A; 58 FR 35338, June 19, 1993
	<i>Process Safety Management of Highly Hazardous Chemicals</i>	includes explosive properties but nothing specific to PETN and/or CO	29 CFR 1910.119
	<i>Explosives</i>	nothing specific to PETN and/or CO	29 CFR 1910.109
	<i>Guidelines for Safety with Hazardous Chemicals</i>	nothing specific to PETN and/or CO	29 CFR 1910.119, Appendix C
National Research Council	<i>Emergency Exposure Guidance Level (EEGL) and CEGLs</i>	1 hr EEGL 400 ppm	
		24 hr EEGL 50 ppm	
		90-day CEGL 20 ppm	NRC 1994
National Institute of Occupational Safety and Health	<i>Recommended Exposure Levels (RELs)</i>		NIOSH 1992
		35 ppm (40 mg/m ³) 8 hr Time Weighted Average	
		200 ppm (229 mg/m ³) Ceiling Limit Health Effect: Cardiovascular	
Department of Interior	None identified		

(continued)

Table 4-1. (continued)

Agency	Description	Information	Reference
<u>ORGANIZATIONS</u>			
American Conference of Governmental Industrial Hygienists (ACGIH)	25 ppm	(29 mg/m ³)	ACGIH 1995
	Short-term Exposure Limit (STEL)	none	
	Ceiling Limit	none	
American Industrial Hygiene Association (AIHA)	<i>Workplace Environmental Exposure Level (WEEL)</i>	None listed for CO	AIHA
American Petroleum Institute (API)	<i>Recommended Procedures (RP)</i>	None specific to CO	API 1999
	RP 750 Management of Process Hazards		
	RP 2220 Improving Owner and Contractor Safety Requirements (http://www.api.org)		
<u>STATE AIR QUALITY STANDARDS</u>			
	<i>Acceptable Ambient Concentration [health-based] Guidelines or Standards</i>		
Arizona		3.5 x 10 ¹ Fg/m ³ 1 hr	NATICH, 1992
Arizona-Pima Co		1.0 x 10 ¹ Fg/m ³ 8 hr 4.0 x 10 ¹ Fg/m ³ annual	NATICH, 1992
Connecticut		1.0 x 10 ⁴ Fg/m ³ 8 hr	NATICH, 1992
Nevada		1.3 x 10 ⁰ Fg/m ³ 8 hr	NATICH, 1992

5.0 Findings and Recommendations

The analysis involved in preparation of this report has shown that CO is a potential risk at all oil wells when perforation involves modern, high explosives. The efforts are summarized below.

- # Theoretical models, laboratory and field testing show that CO is a byproduct of explosives detonation that cannot be avoided.
- # Quantitative estimates of CO amounts are provided which can be used in a qualitative way to evaluate CO risks.
- # Exposures to CO, even briefly, at levels estimated by ambient modeling are of serious concern.
- # Safety procedures presently used in the oil industry could be more broadly applied to minimize CO risks from well perforation.
- # CO is not routinely monitored and should be during well perforation operations

Since this report is based on screening level modeling and information review, there may be a need for followup studies. Suggested monitoring and testing are suggested in Section 5.3.

5.1 Hazard Assessment

A range of potential CO amounts and concentrations in the perforated wellbore have been identified for perforation byproducts. CHEETAH modeling, thermochemistry and laboratory testing of explosives, the testing of the Goodman well, and various published reports of CO measurements help build the case that CO is not an aberration of oil well perforation, but rather an inherent element in the petroleum industry's use of explosives.

Ambient air dispersion modeling suggests that releases of concentrated CO, at least in the volume and weights predicted by CHEETAH, are quickly diluted by the flow of air past a release point. In cases where there is practically no air flow, as was the case at Seacliff (release to a cellar), dilution of CO and other gases takes place much more slowly. Though no modeling was performed to estimate potential exposures in a confined space, the immediate hazard associated with breathing air containing CO at concentrations far above lethal levels must be kept in mind. Safety procedures need to be implemented or maintained anytime there is a potential that a gas is released containing CO in concentrations on the order of 1,000 ppm or greater.

It could be suggested that in assessing the hazards from perforation one look at two general scenarios. The first one is the situation where there is a perforation “upset” or unanticipated release of detonation gases. Concentrations of CO in the undiluted detonation gases may be two to three orders of magnitude higher than levels which are of immediate health concern or particularly levels set by regulatory agencies to keep workers from acute, harmful effects, i.e., measured and estimated CO concentrations of 10,000 to 500,000 ppm versus occupational protective levels from 50 to 400 ppm. It is very clear from Section 3, Hazard Identification, that if a person is exposed briefly to CO from well perforation in undiluted or in moderately diluted concentrations (greater than 1200 ppm), the resulting health impact is immediate and lethal.

The second scenario might involve the normal escape of well gases from the valves, seals, and flanges found on a well, particularly in situations where pressures from the geologic structures are greater than the pressure maintained in the well (underbalanced condition). No reports were identified that provided CO monitoring results from these more routine, post-perforation operations. If slower, unknown releases of CO occur and unprotected workers are exposed to CO levels from 100 to 500 ppm for periods of an hour or two, there is a clear risk that COHb levels would require exposed individuals to require medical attention. Ambient concentrations in this range were estimated for the types of explosives used in perforation.

Loss of CO to fluids and petroleum reservoirs may influence potential CO releases. Though temperature and pressure do affect solubility, the physical conditions in the perforation zone likely play a minor role in the CO released at the wellhead. Fluids and gases released from a valve or flow line quickly reach ambient conditions, meaning the estimates of CO volume and concentration are best performed for standard conditions. Evidence from monitoring and modeling of CO from well perforation suggests that the fraction of CO that stays dissolved in fluids is relatively small.

CO is a very well characterized toxin, and despite the very limited literature base for human exposure to CO from use of explosives, there is a risk associated with perforation operations. The likelihood that a combination of events would lead to release or existence of CO in the breathing space of oil rig workers may be small, but the toxic, potentially fatal, consequences of such exposure demands that the health impacts of CO exposure and associated risks be understood.

5.2 Review of CO Control Options and Recommendation

As previously stated, this report shows that CO is a significant fraction of detonation gases from well perforation and that these levels of contamination are extremely toxic to those directly or closely exposed. However, it is the case that exposure to very toxic levels of CO is uncommon and the risks of exposure at hazardous levels can be kept acceptably low by applying reasonable control measures in practice.

For all those involved in well perforation, there is a need to maintain appropriate operational and safety procedure for all perforation activities. As with other toxic and hazardous gases associated with petroleum wells, e.g., H₂S and methane, the oil industry and its contractors must be committed to carry out proper health and safety procedures, because of the *potential* for CO releases.

Lacking options in reducing the amount of CO generated, the industry could rely on well proven procedures, equipment, training, and information to reduce the potential for CO exposure. The primary elements of a CO risk reduction program for perforation exercises would include

- # pressure testing lubricator, diverter connections and line to formation pressure plus safety factor prior to running in well with explosives;
- # maintaining proper pressures in the wellbore;
- # installing and using flow lines to divert gases and fluids away from work areas;
- # educating all personnel working at a well head to the fact that CO is a major byproduct of the perforating explosives;
- # training personnel, providing respiratory equipment, harnesses and other safety equipment for accidents; and
- # monitoring for CO in areas where wellbore gases could be released.

It is not anticipated that special equipment or operations need to be developed or transferred from other industries to reduce risks to the lowest possible level. Personnel should be trained to recognize when individuals are acutely exposed and how to treat and care for the exposed to allow for the best possible recovery.

5.3 Need for Monitoring under Test Conditions

As demonstrated in this report, planned monitoring for CO during well perforation has only been reported on one known occasion, as described in Section 2.3.2. The results of this test were very important and have been used in the court case related to the accident which caused fatalities. On other occasions, monitoring occurred in response to unanticipated releases (see Section 2.3.3). It would be valuable to have systematic monitoring results that could lead to safer and, possibly, more efficient perforation operations. Some potential uses of such information are described below.

Lawrence Livermore National Laboratories has developed the CHEETAH computer model to predict the results of explosions. However, one must keep in mind that the CHEETAH model was not designed specifically for well perforation scenarios, but for defense applications. Therefore, the framework of the model has limited representativeness of perforation explosions. These limitations (or uncertainties) include

- # CO generation rates in an oxygen-deprived environment, such as downhole, can only be estimated by excluding the generation of CO₂ (the other oxidation product) from the model.

- # Quenching of the detonation prior to complete combustion to simulate borehole conditions is not an option.
- # Under- and over-balance conditions cannot be simulated
- # CO generation cannot be predicted temporally (i.e., one cannot manipulate the number of explosions over time)
- # CHEETAH is able to account for explosions in confined spaces; however, manipulation of the model for this purpose needs further study
- # CHEETAH can predict not only a standard detonation, but also detonation trigger by guns; however, the representativeness of CHEETAH's gun assumptions relative to a HEG, for example, are uncertain.

New CO monitoring tests could validate and calibrate the kind of information that CHEETAH predicts.

Laboratory or field testing of well perforation would support the calibration and modification of thermodynamic models to better suit the oil industry. Additional theoretical and laboratory investigations into the relationship between perforation systems (guns), conditions, and temporal and configurational parameters would also be valuable. As the industry improves petroleum extraction efficiency, in part due to more extensive perforation and in part due to more powerful configurations of explosives, it would be of considerable value to be able to predict potential CO volumes and amounts and, thereby more fully quantify the potential risks of CO exposure, which this study has addressed in a preliminary manner.

6.0 References

- Akhavan, J. 1998. Thermochemistry of Explosives, in *The Chemistry of Explosives*. The Royal Society of Chemistry, Cambridge, England.
- Allen, T. and A. Roberts. 1993. Perforating Oil and Gas Wells, in *Production Operation, Volume 1*. 4th edition. Oil and Gas Consultants International, Inc. Tulsa, OK.
- American Council of Governmental Industrial Hygienists(ACGIH). 1995. Threshold Limit Values (TLVs) for Chemical Substances and Physical Agents. American Council of Governmental Industrial Hygienists. Cincinnati, OH.
- American Petroleum Institute (API). 1999. <http://www.api.com>
- American Petroleum Institute. 1991. API RP-43: "Recommended Practices for Evaluation of Well Perforators," Fifth Edition (Jan. 1991).
- American Petroleum Institute. 1994. API RP-67: "Recommended Practices for Oilfield Explosives Safety," First Edition (March 1, 1994).
- Auger, P.L. et al. 1999. "An Unusual Case of Carbon Monoxide Poisoning". *Environmental Health Perspectives*, Vol. 107, No. 7, July 1999. Pp. 603-605
- Balzan M.V., G. Agius, and D.A. Galea. 1996. Carbon monoxide poisoning: Easy to treat but difficult to recognize. *Postgrad Med J*. 72(850):470-473.
- Behrmann, L.A. and G. McDonald. 1995. Underbalance or Extreme Overbalance. *SPE Production and Facilities*.
- Benaissa, M.L., F. Lapostolle, S.W. Borron, and F.J. Baud. 1999. Delayed transient loss of consciousness in acute carbon monoxide intoxication. *Hum Exp Toxicol*. 18(10):642-643.
- Bennion D., F. Thomas, R. Bletz, and D. Bennion. 1998. Underbalanced drilling: Praises and perils. *SPE Drilling and Completion* 12:214-221.
- CHEETAH. 2000. CHEETAH users manual and program. Lawrence Livermore National Laboratories, U. S. Department of Energy, Lawrence, California.

- Chang, J. C. and J. Kathy. 1997: OCD5: User's Guide for Offshore and Coastal Dispersion (OCD) Model Version 5. Earth Tech, Inc., Concord, MA, prepared for U.S. Department of the Interior, Minerals Management Service, Gulf of Mexico OCS Region, under contract no. 1435-03-96-PO-51307.
- Coric V., D.A. Oren, F.A. Wolkenberg, and R.E. Kravitz. 1998. Carbon monoxide poisoning and treatment with hyperbaric oxygen in the subacute phase. *J Neurol Neurosurg Psychiatry*. 65(2):245-247.
- Crawford H R. 1989. Underbalanced perforating design. SPE, p.19749.
- Deitchman, S., J. Decker, L. Santis. 1998. "A novel source of carbon monoxide poisoning: Explosives used in construction." *Annals of Emergency Medicine*, Vol. 32, No. 3, September 1998, Part 1. pp. 381-384.
- Economides, M.J., L.T. Watters, and S. Dunn-Norman, eds. 1988. *Petroleum Well Construction*. John Wiley and Sons Chichester, England.
- Ellenhorn M.J. and D.G. Barceloux. 1988. Airborne Toxins. In: *Medical Toxicology Diagnosis and Treatment of Human Poisoning*. Elsevier, New York, pp. 820-827.
- Environmental Protection Agency(EPA). 2000. Support Center for Regulatory Air Models. Air Quality Planning and Standards, U.S. Environmental Protection Agency, <http://www.epa.gov/scram001/>.
- Halleck, P. 1997. Recent advances in understanding perforator penetration and flow performance. *SPE Drilling and Completion* 12:19-26.
- Halliburton. 1998. API RP-43 5th edition. Data Summary, 8/21/98. The Halliburton Company, Houston.
- King G E, Anderson A, Bingham M. 1986. A field study of underbalance pressure necessary to obtain clean perforation using tubing-conveyed perforating. *J Pet Tech* 38(7):662-664.
- Lacey D.J. 1981. Neurologic sequelae of acute carbon monoxide intoxication. *Am J Dis Child*. 135(2):145-147.
- Litzinger, T., F. Fetherolf, Y. Lee, and C. Tang. 1995. Study of the gas-phase chemistry of RDX: Experiments and modeling. *Journal of Propulsion and Power* 11(4): 698-703.
- Marius-Nunez, A.L., 1990. Myocardial infarction with normal coronary arteries after acute exposure to carbon monoxide. *Chest*. 97(2):491-494.

- Miró O., J. Casademont, A. Barrientos, A. Urbano-Marquez, and F. Cardellach. 1998. Mitochondrial cytochrome c oxidase inhibition during acute carbon monoxide poisoning. *Pharmacol Toxicol.* 82(4):199-202.
- Miró O., J.R. Alonso, J. Casademont, D. Jarreta, A. Urbano-Marquez, and F. Cardellach. 1999. Oxidative damage on lymphocyte membranes is increased in patients suffering from acute carbon monoxide poisoning. *Toxicol Lett.* 110(3):219-223.
- Mitchell, W.J. and J.C. Suggs. "Emission Factors for the Disposal of Energetic Materials by Open Burning and Open Detonation (OB/OD)." U.S. Environmental Protection Agency, MD-46, Research Triangle Park, NC 27711. August 1998. (This emission factor database was created using data collected by the U.S. Department of Defense.)
- National Air Toxics Clearinghouse (NATICH). 1992. NATICH Database Report on State, Local, and EPA Air Toxics Activities, September 1992. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC.
- National Institute of Occupational Safety and Health (NIOSH). 1992. Recommendations for Occupational Safety and Health - Compendium of Policy Documents and Statements. Table 1 - NIOSH Recommended Safety and Health Standards for Hazardous Agents in the Workplace. NIOSH. Cincinnati, OH.
- National Research Council (NRC). 1994. Emergency Exposure Guidance Limits. Committee on Toxicology, National Research Council, National Academy of Sciences, Washington, DC.
- Ornellas D. 1974. The Heat and Products of Detonation in a Calorimeter of CNO, HNO, CHNF, CHNO, CHNOT, and CHNOSi Explosives. *Combustion and Flame* 23:37-46.
- Owen Tools. 2000. Perforation Charge Cross-Section. <http://www.owenstools.com/API/Hydrocode/default.htm>
- Petrash, D., A. Graff, and J. Trantham. 1999. Proactive Approach to Well Construction Safety in Alaska's Kuparuk River Field. *SPE Drill and Completion.* 14(3):157-161.
- Ree, F, W. Pitz, M. van Thief, and P. Souers. 1996. Overabundance of carbon monoxide in calorimetry tests. *J Phys Chem* 100:5761-5765.
- Schlumberger. 2000. Enerjet system. http://www.connect.slb.com/inserts.cfm?id=id14737&fn=connect/completion/Perforating_Data_Sheets/2-18_rpes.html).
- Schlumberger. 1993. Perforating Services. Schlumberger.Wireline and Testing, Houston, TX.
- Schulman, L.S., D.G. Strimaitis, and J.S. Scire. 1997. Addendum to ISC3 User's Guide, The Prime Plume Rise and Building Downwash Model. Earth Tech, Inc., Concord, MA.

- Thom, S.R. and L.W. Keim. 1989. Carbon monoxide poisoning: a review of epidemiology, pathophysiology, clinical findings, and treatment options including hyperbaric oxygen therapy. *J Toxicol Clin Toxicol.* 27(3):141-156.
- Velsko, C.A., et al. 1999. Emissions Characterization in the Contained Underground Demilitarization Laboratory at the Nevada Test Site. U.S. Department of Energy, Lawrence Livermore National Laboratory. Submitted to the *Fifth Conference on Life Cycles of Energetic Materials*, Orlando, FL. September 26-29, 1999.
- Wilson R.C., P.J. Sanders, and G. Smith. 1998. An epidemiological study of acute carbon monoxide poisoning in the West Midlands. *Occup Environ Med.* 55(11):723-728.
- Wright W. 1995. Memorandum: "Incident Report" for Goodman 1. To: Barry McMahan, Well Files, and Division of Oil and Gas, State of California, Ventura. September 20, 1995.

Appendix A

Modeling of Carbon Monoxide Generation Using CHEETAH

<u>Section</u>	<u>Explosive</u>	<u>Conditions</u>
A1	HMX	Standard Detonation
A2	HMX	Standard Detonation, without CO ₂ among byproduct
A3	RDX	Gun
A4	RDX	Gun, Confined Space
A5	RDX	Gun, Confined Space, without CO ₂ among byproduct
A6	RDX	Standard Detonation
A7	RDX	Standard Detonation, without CO ₂ among byproduct
A8	HNS	Standard Detonation
A9	HNS	Standard Detonation, without CO ₂ among byproduct
A10	PYX	Standard Detonation
A11	PYX	Standard Detonation, without CO ₂ among byproduct
A12	PETN	Gun, without CO ₂ among byproduct
A13	PETN	Gun, Confined Space
A14	PETN	Gun, Confined Space, without CO ₂ among byproduct
A15	PETN	Standard Detonation
A16	PETN	Standard Detonation, without CO ₂ among byproduct
A17	PETN	Standard Detonation, Confined Space
A18	PETN	Standard Detonation, Confined Space, without CO ₂ among byproduct

A1. HMX Standard Detonation

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
hmx	100.00	100.00	100.00	17866	155.47	0.000	296.17	c4h8n8o8

Heat of formation = 60.323 cal/gm
 Standard volume = 0.525 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 60.310 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 296.168 g/mol

Input>standard run, rho, 1.905000

The initial damping was too small

Undertaking a gradient line search instead

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.524934 cc/gm, E0 = 60.310073 cal/gm

Using 171946 ATM as a lower bound for the C-J pressure

Using 429865 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 9.30083e+003 m/s

The particle velocity = 2.22191e+003 m/s

The speed of sound = 7.07892e+003 m/s

P0 = 1 atm, V0 = 0.52493 cc/gm, E0 = 60.31007 cal/gm

Reference state = reactants

H(R) = H-60.32, E(R) = E-60.31, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	388533.4	0.3995	4113.2	4349.37	590.00	1.660	0.3839

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.350e+001	3.999e+000
h2o Gas	1.350e+001	3.999e+000

co2	Gas	6.418e+000	1.901e+000
co	Gas	6.565e-001	1.944e-001
no	Gas	7.167e-003	2.123e-003
ch2o2	Gas	3.959e-003	1.172e-003
o2	Gas	1.938e-003	5.740e-004
ch4	Gas	1.764e-004	5.224e-005
c2h4	Gas	1.224e-004	3.625e-005
ch3oh	Gas	4.698e-005	1.391e-005
h2	Gas	4.641e-005	1.374e-005
h3n	Gas	1.617e-005	4.789e-006
ch2o	Gas	5.138e-007	1.522e-007
ch3	Gas	8.941e-011	2.648e-011
c2h6	Gas	8.760e-013	2.595e-013
no2	Gas	2.695e-014	7.981e-015
*c	solid	6.427e+000	1.904e+000
Total	Gas	3.409e+001	1.010e+001
Total	Cond.	6.427e+000	1.904e+000

The C-J Adiabatic

Reference state = reactants

H(R) = H-60.32, E(R) = E-60.31, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	159287.4	0.5249	3224.2	1848.12	-176.87	1.660	0.5042

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.350e+001 4.000e+000
h2o	Gas	1.346e+001 3.987e+000
co2	Gas	5.516e+000 1.634e+000
co	Gas	2.494e+000 7.385e-001
ch2o2	Gas	1.142e-002 3.382e-003
ch4	Gas	1.078e-002 3.193e-003
h2	Gas	4.151e-003 1.229e-003
c2h4	Gas	2.445e-003 7.242e-004
h3n	Gas	9.784e-004 2.898e-004
no	Gas	7.460e-004 2.209e-004
ch3oh	Gas	5.920e-004 1.753e-004
ch2o	Gas	4.500e-005 1.333e-005
o2	Gas	2.162e-005 6.402e-006
ch3	Gas	1.148e-007 3.400e-008
c2h6	Gas	1.645e-008 4.872e-009
no2	Gas	3.976e-013 1.177e-013
*c	solid	5.468e+000 1.619e+000
Total	Gas	3.501e+001 1.037e+001
Total	Cond.	5.468e+000 1.619e+000

Reference state = reactants

$$H(R) = H-60.32, E(R) = E-60.31, S(R) = S- 0.00$$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	36182.4	0.8447	2145.0	-34.67	-774.87	1.660	0.8284

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.349e+001	3.996e+000
h2o Gas	1.263e+001	3.740e+000
co2 Gas	4.827e+000	1.430e+000
co Gas	4.708e+000	1.394e+000
ch4 Gas	3.095e-001	9.166e-002
h2 Gas	1.973e-001	5.843e-002
h3n Gas	2.562e-002	7.587e-003
ch2o2 Gas	9.036e-003	2.676e-003
c2h4 Gas	5.163e-003	1.529e-003
ch3oh Gas	1.297e-003	3.840e-004
ch2o Gas	6.594e-004	1.953e-004
c2h6 Gas	3.949e-005	1.170e-005
ch3 Gas	8.115e-006	2.403e-006
no Gas	3.760e-006	1.114e-006
o2 Gas	4.260e-009	1.262e-009
no2 Gas	3.600e-014	1.066e-014
*c solid	3.639e+000	1.078e+000
Total Gas	3.621e+001	1.072e+001
Total Cond.	3.639e+000	1.078e+000

A2. HMX Standard Detonation, without CO₂

Input>reject, co2

Input>composition, hmx, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
hmx	100.00	100.00	100.00	17866	155.47	0.000	296.17	c4h8n8o8

Heat of formation = 60.323 cal/gm
 Standard volume = 0.525 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 60.310 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 296.168 g/mol

Input>standard run, rho, 1.905000

The initial damping was too small

Undertaking a gradient line search instead

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.524934 cc/gm, E0 = 60.310073 cal/gm

Using 194389 ATM as a lower bound for the C-J pressure

Using 485973 ATM as an upper bound for the C-J pressure

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The initial P bracket of : 1.943891e+005, 4.859727e+005 did not work

The C-J function values were: 1.140831e-001, 4.445527e-002

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

New upper pressure limit = 585972.7

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 9.05863e+003 m/s

The particle velocity = 3.27608e+003 m/s

The speed of sound = 5.78255e+003 m/s

P0 = 1 atm, V0 = 0.52493 cc/gm, E0 = 60.31007 cal/gm

Reference state = reactants

H(R) = H-60.32, E(R) = E-60.31, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	557950.4	0.3351	3723.1	5810.52	1282.63	1.557	0.3196

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.350e+001	3.999e+000
n2 Gas	1.345e+001	3.983e+000
o2 Gas	5.546e+000	1.642e+000
co Gas	2.297e+000	6.802e-001
no Gas	1.143e-001	3.385e-002
ch2o2 Gas	3.197e-003	9.470e-004
h2 Gas	2.979e-009	8.822e-010
ch3oh Gas	2.170e-009	6.426e-010
ch4 Gas	1.746e-010	5.170e-011
ch2o Gas	1.382e-010	4.092e-011
h3n Gas	1.036e-010	3.069e-011
c2h4 Gas	5.138e-011	1.522e-011
no2 Gas	1.541e-015	4.564e-016
ch3 Gas	1.084e-018	3.212e-019
c2h6 Gas	1.154e-024	3.417e-025
*c solid	1.121e+001	3.319e+000
Total Gas	3.491e+001	1.034e+001
Total Cond.	1.121e+001	3.319e+000

The C-J Adiabatic

Reference state = reactants

$$H(R) = H-60.32, E(R) = E-60.31, S(R) = S- 0.00$$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	166109.3	0.5249	2438.1	1790.26	-321.46	1.557	0.5249

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.351e+001	4.000e+000
h2o Gas	1.348e+001	3.991e+000
co Gas	1.348e+001	3.991e+000
ch2o2 Gas	2.961e-002	8.770e-003
no Gas	5.861e-004	1.736e-004
o2 Gas	2.669e-004	7.904e-005
h2 Gas	6.706e-006	1.986e-006
ch4 Gas	1.045e-006	3.094e-007
ch3oh Gas	6.566e-007	1.945e-007
ch2o Gas	4.234e-007	1.254e-007
h3n Gas	3.153e-007	9.338e-008
c2h4 Gas	5.538e-008	1.640e-008
ch3 Gas	4.463e-013	1.322e-013
no2 Gas	2.753e-014	8.155e-015
c2h6 Gas	6.259e-016	1.854e-016
*c solid	1.108e-003	3.280e-004
Total Gas	4.049e+001	1.199e+001
Total Cond.	1.108e-003	3.280e-004

Reference state = reactants
 H(R) = H-60.32, E(R) = E-60.31, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	111048.3	0.5838	2145.0	1054.48	-515.62	1.557	0.5838

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.351e+001	4.000e+000
co Gas	1.348e+001	3.992e+000
h2o Gas	1.348e+001	3.992e+000
ch2o2 Gas	2.856e-002	8.459e-003
no Gas	7.402e-005	2.192e-005
h2 Gas	4.113e-005	1.218e-005
o2 Gas	8.071e-006	2.390e-006
ch4 Gas	6.662e-006	1.973e-006
h3n Gas	1.998e-006	5.917e-007
ch2o Gas	1.576e-006	4.666e-007
ch3oh Gas	1.496e-006	4.432e-007
c2h4 Gas	1.300e-007	3.849e-008
ch3 Gas	4.589e-012	1.359e-012
c2h6 Gas	3.983e-014	1.180e-014
no2 Gas	1.427e-014	4.225e-015
*c solid	2.097e-005	6.209e-006
Total Gas	4.049e+001	1.199e+001
Total Cond.	2.097e-005	6.209e-006

A3. RDX gun

Product library title: bkwc
 Executing library command: gas eos, bkwc
 Executing library command: set, bkwc, alpha, 0.499123809964
 Executing library command: set, bkwc, beta, 0.402655787895
 Executing library command: set, bkwc, theta, 5441.84607543
 Executing library command: set, bkwc, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

Input>gun, 0.500000, 0.250000, 1.000000

GUN calculation:

WARNING: Results will not match BLAKE -- the virial EOS is not being used

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
The initial damping was too small								
Undertaking a gradient line search instead								
1.)	0.5000	4086.3	1374.7	1376.23	24.688	0.999	1.192	1.998
2.)	0.7500	3965.5	2729.5	1332.43	24.746	0.845	1.191	2.731
3.)	1.0000	3831.2	4679.7	1277.57	24.934	0.727	1.192	3.663

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
n2	Gas	1.346e+001	1.347e+001	1.346e+001
co	Gas	1.088e+001	1.128e+001	1.142e+001
h2o	Gas	1.081e+001	1.129e+001	1.172e+001
h2	Gas	2.628e+000	2.068e+000	1.338e+000
co2	Gas	2.607e+000	2.186e+000	1.895e+000
no	Gas	6.630e-002	2.122e-002	6.623e-003
h3n	Gas	3.040e-002	6.044e-002	8.868e-002
ch2o2	Gas	1.163e-002	2.051e-002	3.008e-002
ch2o	Gas	4.817e-003	8.024e-003	9.758e-003
o2	Gas	4.526e-003	6.951e-004	1.120e-004
ch4	Gas	9.321e-004	1.242e-002	1.225e-001
ch3	Gas	2.691e-004	7.613e-004	1.314e-003
ch3oh	Gas	1.179e-004	9.024e-004	4.986e-003
no2	Gas	8.303e-006	4.257e-007	1.474e-008
c2h4	Gas	4.463e-006	2.500e-004	9.900e-003
c2h6	Gas	1.949e-008	1.223e-006	3.642e-005
*c	solid	0.000e+000	0.000e+000	0.000e+000
Total Gas		4.051e+001	4.041e+001	4.011e+001
Total Cond.		0.000e+000	0.000e+000	0.000e+000

Input>library file, blake.chl

Product library title: the blake product library

Executing library command: gas eos, virial

Input>composition, rdx, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

```
Input>gas eos, virial
Input>gun, 0.500000, 0.250000, 1.000000
GUN calculation:
```

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
The initial equation error was huge: 10110.990602								
1.)	0.5000	4167.4	1260.2	1408.32	24.604	0.882	1.247	1.790
2.)	0.7500	4190.5	2450.5	1397.22	24.937	0.763	1.275	2.339
3.)	1.0000	4181.4	3976.0	1356.18	25.636	0.659	1.303	2.932

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
n2	Gas	1.338e+001	1.327e+001	1.298e+001
co	Gas	1.033e+001	1.002e+001	9.057e+000
h2o	Gas	1.002e+001	1.020e+001	1.009e+001
h2	Gas	3.070e+000	2.588e+000	1.868e+000
co2	Gas	3.026e+000	2.997e+000	3.086e+000
oh	Gas	3.080e-001	1.908e-001	1.206e-001
h	Gas	1.491e-001	7.669e-002	3.611e-002
no	Gas	1.236e-001	8.465e-002	6.292e-002
nh3	Gas	5.369e-002	1.504e-001	3.147e-001
cho	Gas	4.204e-002	8.846e-002	1.518e-001
hcn	Gas	3.307e-002	1.073e-001	2.508e-001
formac	Gas	3.134e-002	1.238e-001	4.126e-001
hnco	Gas	2.394e-002	1.044e-001	3.689e-001
ch2o	Gas	1.351e-002	4.459e-002	1.104e-001
nh2	Gas	9.784e-003	1.699e-002	2.343e-002
o	Gas	9.147e-003	3.653e-003	1.593e-003
o2	Gas	8.556e-003	3.440e-003	1.689e-003
hno	Gas	3.234e-003	4.278e-003	5.504e-003
nh	Gas	1.674e-003	1.863e-003	1.777e-003
h2o2	Gas	1.221e-003	1.470e-003	1.780e-003
n2o	Gas	1.107e-003	1.928e-003	3.546e-003
ho2	Gas	1.017e-003	7.811e-004	6.554e-004
nco	Gas	9.930e-004	2.808e-003	6.832e-003
n	Gas	6.321e-004	4.451e-004	2.950e-004
ch3	Gas	6.019e-004	2.679e-003	7.034e-003
cn	Gas	5.575e-004	1.324e-003	2.388e-003
ch4	Gas	3.494e-004	1.758e-003	4.766e-003
hno2	Gas	3.261e-004	5.227e-004	9.008e-004
no2	Gas	2.410e-004	2.441e-004	2.925e-004
ketene	Gas	1.962e-004	2.228e-003	1.490e-002
ch2oh	Gas	1.433e-004	7.727e-004	2.718e-003
ch4o	Gas	1.116e-004	9.401e-004	4.778e-003
c2h2	Gas	8.181e-005	7.822e-004	3.876e-003
ch2	Gas	7.684e-005	2.209e-004	3.999e-004
ch3cn	Gas	2.866e-006	9.113e-005	1.330e-003
c	Gas	1.600e-006	1.880e-006	1.631e-006
c2h4	Gas	1.055e-006	1.404e-005	7.564e-005
c(s)	solid	0.000e+000	0.000e+000	0.000e+000
Total	Gas	4.064e+001	4.010e+001	3.901e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000

A4. RDX, gun, confined space

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

Input>gun, 0.500000, 0.250000, 1.000000

GUN calculation:

WARNING: Results will not match BLAKE -- the virial EOS is not being used

Rho	Temp	Pressure	Impetus	Mol Wt.	Covol	Frozen	Phi
g/cc	K	MPa	J/g	Gas	cc/g	Cp/Cv	

The initial damping was too small

Undertaking a gradient line search instead

1.)	0.5000	4086.3	1374.7	1376.23	24.688	0.999	1.192	1.998
2.)	0.7500	3965.5	2729.5	1332.43	24.746	0.845	1.191	2.731
3.)	1.0000	3831.2	4679.7	1277.57	24.934	0.727	1.192	3.663

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
n2	Gas	1.346e+001	1.347e+001	1.346e+001
co	Gas	1.088e+001	1.128e+001	1.142e+001
h2o	Gas	1.081e+001	1.129e+001	1.172e+001
h2	Gas	2.628e+000	2.068e+000	1.338e+000
co2	Gas	2.607e+000	2.186e+000	1.895e+000
no	Gas	6.630e-002	2.122e-002	6.623e-003
h3n	Gas	3.040e-002	6.044e-002	8.868e-002
ch2o2	Gas	1.163e-002	2.051e-002	3.008e-002
ch2o	Gas	4.817e-003	8.024e-003	9.758e-003
o2	Gas	4.526e-003	6.951e-004	1.120e-004
ch4	Gas	9.321e-004	1.242e-002	1.225e-001
ch3	Gas	2.691e-004	7.613e-004	1.314e-003
ch3oh	Gas	1.179e-004	9.024e-004	4.986e-003

```

no2 Gas 8.303e-006 4.257e-007 1.474e-008
c2h4 Gas 4.463e-006 2.500e-004 9.900e-003
c2h6 Gas 1.949e-008 1.223e-006 3.642e-005
*c solid 0.000e+000 0.000e+000 0.000e+000

Total Gas 4.051e+001 4.041e+001 4.011e+001
Total Cond. 0.000e+000 0.000e+000 0.000e+000
Input>point, p, 100000.000000, t, 3000.000000

```

Reference state = reactants
H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	100000.0	0.6203	3000.0	1153.03	-349.26	1.702	0.6024

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.350e+001	2.999e+000
h2o Gas	1.330e+001	2.954e+000
co2 Gas	4.602e+000	1.022e+000
co Gas	4.472e+000	9.934e-001
ch4 Gas	6.281e-002	1.395e-002
h2 Gas	3.302e-002	7.335e-003
ch2o2 Gas	1.666e-002	3.701e-003
c2h4 Gas	8.878e-003	1.972e-003
h3n Gas	6.042e-003	1.342e-003
ch3oh Gas	1.732e-003	3.848e-004
no Gas	3.370e-004	7.486e-005
ch2o Gas	3.217e-004	7.146e-005
o2 Gas	3.922e-006	8.712e-007
ch3 Gas	2.990e-006	6.642e-007
c2h6 Gas	1.110e-006	2.466e-007
no2 Gas	1.649e-012	3.662e-013
*c solid	4.332e+000	9.623e-001

```

Total Gas 3.601e+001 7.998e+000
Total Cond. 4.332e+000 9.623e-001
Input>explosion, rho, 1.000000

```

The Constant Volume Explosion State:

Reference state = reactants
H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	46185.2	1.0000	3831.2	1118.50	0.00	1.993	1.0000

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.346e+001	2.989e+000
h2o Gas	1.172e+001	2.603e+000
co Gas	1.142e+001	2.537e+000

co2	Gas	1.895e+000	4.208e-001
h2	Gas	1.338e+000	2.972e-001
ch4	Gas	1.225e-001	2.722e-002
h3n	Gas	8.868e-002	1.970e-002
ch2o2	Gas	3.008e-002	6.683e-003
c2h4	Gas	9.900e-003	2.199e-003
ch2o	Gas	9.758e-003	2.167e-003
no	Gas	6.623e-003	1.471e-003
ch3oh	Gas	4.986e-003	1.107e-003
ch3	Gas	1.314e-003	2.918e-004
o2	Gas	1.120e-004	2.489e-005
c2h6	Gas	3.642e-005	8.089e-006
no2	Gas	1.474e-008	3.274e-009
*c	solid	0.000e+000	0.000e+000
Total	Gas	4.011e+001	8.908e+000
Total	Cond.	0.000e+000	0.000e+000

A5. RDX, gun, confined space, without CO₂ byproduct

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

Input>reject, co2

Input>composition, rdx, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

Input>gun, 0.500000, 0.250000, 1.000000

GUN calculation:

WARNING: Results will not match BLAKE -- the virial EOS is not being used

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.5000	3987.0	1324.5	1351.44	24.530	0.980	1.197	1.960
2.)	0.7500	3912.2	2637.3	1321.40	24.617	0.832	1.195	2.661
3.)	1.0000	3794.2	4568.4	1278.80	24.669	0.720	1.197	3.573

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
co	Gas	1.349e+001	1.348e+001	1.347e+001
n2	Gas	1.335e+001	1.342e+001	1.346e+001
h2o	Gas	1.295e+001	1.321e+001	1.335e+001
h2	Gas	5.335e-001	2.671e-001	1.143e-001
no	Gas	3.104e-001	1.729e-001	8.224e-002
o2	Gas	1.140e-001	4.973e-002	1.823e-002
ch2o2	Gas	1.613e-002	2.687e-002	3.763e-002
h3n	Gas	2.715e-003	2.680e-003	2.102e-003
ch2o	Gas	1.148e-003	1.166e-003	9.197e-004
no2	Gas	1.970e-004	2.957e-005	2.299e-006
ch4	Gas	8.492e-006	2.597e-005	7.378e-005
ch3oh	Gas	5.693e-006	1.624e-005	3.835e-005
ch3	Gas	4.750e-006	4.223e-006	2.619e-006
c2h4	Gas	8.083e-009	6.412e-008	4.921e-007
c2h6	Gas	7.416e-012	4.036e-011	1.504e-010
*c	solid	0.000e+000	0.000e+000	0.000e+000
Total Gas		4.077e+001	4.062e+001	4.054e+001
Total Cond.		0.000e+000	0.000e+000	0.000e+000

Input>point, p, 100000.000000, t, 3000.000000

Reference state = reactants

H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	100000.0	0.6627	3000.0	1404.09	-200.92	1.766	0.6627

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)	
n2	Gas	1.350e+001	3.000e+000
co	Gas	1.346e+001	2.991e+000
h2o	Gas	1.346e+001	2.990e+000
ch2o2	Gas	4.151e-002	9.221e-003
no	Gas	3.454e-003	7.672e-004
h2	Gas	3.382e-003	7.512e-004
o2	Gas	4.195e-004	9.319e-005
h3n	Gas	1.681e-004	3.733e-005
ch4	Gas	1.571e-004	3.490e-005
ch2o	Gas	8.238e-005	1.830e-005
ch3oh	Gas	4.062e-005	9.024e-006
c2h4	Gas	6.044e-006	1.342e-006
ch3	Gas	2.360e-008	5.242e-009
no2	Gas	1.445e-010	3.210e-011
c2h6	Gas	6.205e-011	1.378e-011
*c	solid	0.000e+000	0.000e+000
Total Gas		4.048e+001	8.991e+000
Total Cond.		0.000e+000	0.000e+000

Input>explosion, rho, 1.000000

The Constant Volume Explosion State:

Reference state = reactants

H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	45087.1	1.0000	3794.2	1091.91	0.00	1.985	1.0000

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.347e+001	2.991e+000
n2 Gas	1.346e+001	2.991e+000
h2o Gas	1.335e+001	2.965e+000
h2 Gas	1.143e-001	2.540e-002
no Gas	8.224e-002	1.827e-002
ch2o2 Gas	3.763e-002	8.358e-003
o2 Gas	1.823e-002	4.050e-003
h3n Gas	2.102e-003	4.669e-004
ch2o Gas	9.197e-004	2.043e-004
ch4 Gas	7.378e-005	1.639e-005
ch3oh Gas	3.835e-005	8.519e-006
ch3 Gas	2.619e-006	5.817e-007
no2 Gas	2.299e-006	5.107e-007
c2h4 Gas	4.921e-007	1.093e-007
c2h6 Gas	1.504e-010	3.341e-011
*c solid	0.000e+000	0.000e+000
Total Gas	4.054e+001	9.004e+000
Total Cond.	0.000e+000	0.000e+000

A6. RDX Standard Detonation

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

Input>standard run, rho, 1.806000

The initial damping was too small

Undertaking a gradient line search instead

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.553710 cc/gm, E0 = 74.251539 cal/gm

Using 153445 ATM as a lower bound for the C-J pressure

Using 383612 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 8.94242e+003 m/s

The particle velocity = 2.15134e+003 m/s

The speed of sound = 6.79108e+003 m/s

P0 = 1 atm, V0 = 0.55371 cc/gm, E0 = 74.25154 cal/gm

Reference state = reactants

H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	342898.5	0.4205	4209.0	4045.07	553.11	1.699	0.4038

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.350e+001	2.999e+000

h2o	Gas	1.350e+001	2.998e+000
co2	Gas	6.172e+000	1.371e+000
co	Gas	1.145e+000	2.544e-001
no	Gas	8.754e-003	1.944e-003
ch2o2	Gas	7.701e-003	1.711e-003
o2	Gas	1.687e-003	3.748e-004
ch4	Gas	6.787e-004	1.507e-004
c2h4	Gas	5.151e-004	1.144e-004
h2	Gas	1.977e-004	4.392e-005
ch3oh	Gas	1.562e-004	3.470e-005
h3n	Gas	6.470e-005	1.437e-005
ch2o	Gas	2.940e-006	6.531e-007
ch3	Gas	1.473e-009	3.273e-010
c2h6	Gas	2.491e-011	5.533e-012
no2	Gas	2.387e-013	5.303e-014
*c	solid	6.179e+000	1.373e+000
Total Gas		3.433e+001	7.626e+000
Total Cond.		6.179e+000	1.373e+000

The C-J Adiabatic

Reference state = reactants

H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	142207.6	0.5537	3298.5	1738.58	-168.38	1.699	0.5345

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2	Gas	1.350e+001
h2o	Gas	1.342e+001
co2	Gas	5.038e+000
co	Gas	3.487e+000
ch4	Gas	2.332e-002
ch2o2	Gas	1.599e-002
h2	Gas	1.037e-002
c2h4	Gas	5.643e-003
h3n	Gas	2.236e-003
ch3oh	Gas	1.168e-003
no	Gas	9.447e-004
ch2o	Gas	1.266e-004
o2	Gas	2.327e-005
ch3	Gas	6.457e-007
c2h6	Gas	1.103e-007
no2	Gas	1.654e-012
*c	solid	4.930e+000
Total Gas		3.550e+001
Total Cond.		4.930e+000

Reference state = reactants

H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	30018.4	0.9307	2145.0	-97.05	-773.62	1.699	0.9193

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.349e+001	2.996e+000
h2o Gas	1.206e+001	2.678e+000
co Gas	5.984e+000	1.329e+000
co2 Gas	4.475e+000	9.940e-001
ch4 Gas	5.006e-001	1.112e-001
h2 Gas	3.573e-001	7.937e-002
h3n Gas	4.041e-002	8.976e-003
ch2o2 Gas	9.789e-003	2.174e-003
c2h4 Gas	8.408e-003	1.868e-003
ch3oh Gas	1.743e-003	3.871e-004
ch2o Gas	1.184e-003	2.630e-004
c2h6 Gas	1.230e-004	2.733e-005
ch3 Gas	2.263e-005	5.026e-006
no Gas	3.647e-006	8.101e-007
o2 Gas	3.423e-009	7.604e-010
no2 Gas	6.381e-014	1.417e-014
*c solid	2.516e+000	5.590e-001
Total Gas	3.692e+001	8.201e+000
Total Cond.	2.516e+000	5.590e-001

A7. RDX standard detonation without CO2 byproduct

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286	h	28.571
n	28.571	o	28.571

The average mol. wt. = 222.126 g/mol

Input>reject, co2

Input>composition, rdx, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
rdx	100.00	100.00	100.00	16496	122.99	0.000	222.13	c3h6n6o6

Heat of formation = 74.265 cal/gm
 Standard volume = 0.554 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 74.252 cal/gm

The elements and percent by mole

c	14.286
h	28.571
n	28.571
o	28.571

The average mol. wt. = 222.126 g/mol

Input>standard run, rho, 1.806000

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.553710 cc/gm, E0 = 74.251539 cal/gm

Using 170730 ATM as a lower bound for the C-J pressure

Using 426826 ATM as an upper bound for the C-J pressure

The C-J function values were: 1.236328e-001, 4.369588e-002

New upper pressure limit = 526825.6

New upper pressure limit = 626825.6

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 9.06829e+003 m/s
 The particle velocity = 3.40551e+003 m/s
 The speed of sound = 5.66278e+003 m/s

P0 = 1 atm, V0 = 0.55371 cc/gm, E0 = 74.25154 cal/gm

Reference state = reactants

H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	550438.6	0.3458	4038.6	5995.27	1385.98	1.624	0.3309

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.350e+001	2.999e+000
n2 Gas	1.342e+001	2.981e+000
o2 Gas	5.056e+000	1.123e+000
co Gas	3.214e+000	7.138e-001
no Gas	1.730e-001	3.842e-002
ch2o2 Gas	6.566e-003	1.458e-003
h2 Gas	2.065e-008	4.588e-009
ch3oh Gas	1.620e-008	3.599e-009
ch4 Gas	1.619e-009	3.597e-010
ch2o Gas	1.260e-009	2.800e-010
h3n Gas	9.043e-010	2.009e-010
c2h4 Gas	6.792e-010	1.509e-010
no2 Gas	2.286e-014	5.078e-015
ch3 Gas	5.842e-017	1.298e-017
c2h6 Gas	1.798e-022	3.994e-023
*c solid	1.029e+001	2.285e+000
Total Gas	3.537e+001	7.856e+000
Total Cond.	1.029e+001	2.285e+000

The C-J Adiabatic

Reference state = reactants

$$H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00$$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	149678.9	0.5537	2631.3	1732.07	-275.08	1.624	0.5537

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.351e+001	3.000e+000
h2o Gas	1.347e+001	2.992e+000
co Gas	1.347e+001	2.992e+000
ch2o2 Gas	3.467e-002	7.701e-003
no Gas	8.287e-004	1.841e-004
o2 Gas	1.776e-004	3.945e-005
h2 Gas	7.194e-005	1.598e-005
ch4 Gas	1.730e-005	3.842e-006
ch3oh Gas	5.884e-006	1.307e-006
h3n Gas	4.345e-006	9.652e-007
ch2o Gas	3.551e-006	7.888e-007
c2h4 Gas	1.347e-006	2.993e-007
ch3 Gas	4.261e-011	9.464e-012
no2 Gas	2.434e-013	5.406e-014
c2h6 Gas	1.874e-013	4.163e-014
*c solid	1.033e-003	2.294e-004
Total Gas	4.048e+001	8.992e+000
Total Cond.	1.033e-003	2.294e-004

Reference state = reactants
 H(R) = H-74.26, E(R) = E-74.25, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	75722.3	0.6704	2145.0	651.78	-577.63	1.624	0.6704

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	1.351e+001	3.000e+000
co Gas	1.348e+001	2.994e+000
h2o Gas	1.348e+001	2.994e+000
ch2o2 Gas	2.889e-002	6.417e-003
h2 Gas	1.945e-004	4.319e-005
no Gas	1.706e-004	3.790e-005
o2 Gas	2.160e-005	4.798e-006
h3n Gas	5.172e-006	1.149e-006
ch2o Gas	4.200e-006	9.330e-007
ch4 Gas	2.004e-006	4.452e-007
ch3oh Gas	6.819e-007	1.515e-007
c2h4 Gas	6.986e-009	1.552e-009
no2 Gas	1.502e-012	3.337e-013
c2h6 Gas	2.118e-014	4.705e-015
*c solid	0.000e+000	0.000e+000
Total Gas	4.049e+001	8.994e+000
Total Cond.	0.000e+000	0.000e+000

A8. HNS standard detonation

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
hns	100.00	100.00	100.00	16969	258.76	0.000	450.24	c14h6n6o12

Heat of formation = 37.690 cal/gm
 Standard volume = 0.575 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 37.676 cal/gm

The elements and percent by mole

c	36.842
h	15.789
n	15.789
o	31.579

The average mol. wt. = 450.236 g/mol
 Input>standard run, rho, 1.740000
 The Newton line search was not successful.
 Undertaking a gradient line search instead
 The initial damping was too small
 Undertaking a gradient line search instead
 The initial damping was too small
 Undertaking a gradient line search instead
 The hugoniot reference state:
 P0 = 1.000000 ATM, V0 = 0.574713 cc/gm, E0 = 37.676109 cal/gm
 Using 100558 ATM as a lower bound for the C-J pressure
 Using 251396 ATM as an upper bound for the C-J pressure
 The C-J point was bracketed in cjbrent
 The CJ state was found in 6 iterations
 The C-J condition

The shock velocity = 7.22201e+003 m/s
 The particle velocity = 1.84531e+003 m/s
 The speed of sound = 5.37670e+003 m/s

P0 = 1 atm, V0 = 0.57471 cc/gm, E0 = 37.67611 cal/gm

Reference state = reactants
 H(R) = H-37.69, E(R) = E-37.68, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	228855.8	0.4279	4039.5	2778.36	406.94	1.520	0.3613

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co2 Gas	8.521e+000	3.836e+000
n2 Gas	6.660e+000	2.999e+000
h2o Gas	6.632e+000	2.986e+000
co Gas	2.929e+000	1.319e+000
ch2o2 Gas	2.164e-002	9.744e-003
no Gas	5.306e-003	2.389e-003
ch4 Gas	2.053e-003	9.241e-004
c2h4 Gas	1.408e-003	6.339e-004
h2 Gas	1.172e-003	5.276e-004
o2 Gas	6.273e-004	2.824e-004
ch3oh Gas	4.466e-004	2.011e-004
h3n Gas	2.516e-004	1.133e-004
ch2o Gas	4.699e-005	2.115e-005
ch3 Gas	8.330e-008	3.750e-008
c2h6 Gas	2.799e-009	1.260e-009
no2 Gas	1.161e-011	5.227e-012
*c solid	1.962e+001	8.833e+000
Total Gas	2.477e+001	1.115e+001
Total Cond.	1.962e+001	8.833e+000

The C-J Adiabatic

Reference state = reactants
 H(R) = H-37.69, E(R) = E-37.68, S(R) = S- 0.00

P	V	T	H(R)	E(R)	S(R)	VGS
---	---	---	------	------	------	-----

	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	93558.6	0.5747	3196.7	1180.92	-121.25	1.520	0.5011

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	6.817e+000	3.069e+000
n2 Gas	6.661e+000	2.999e+000
co2 Gas	6.621e+000	2.981e+000
h2o Gas	6.545e+000	2.947e+000
h2 Gas	2.711e-002	1.220e-002
ch4 Gas	2.525e-002	1.137e-002
ch2o2 Gas	2.297e-002	1.034e-002
c2h4 Gas	5.091e-003	2.292e-003
h3n Gas	3.070e-003	1.382e-003
ch3oh Gas	1.179e-003	5.306e-004
ch2o Gas	5.847e-004	2.633e-004
no Gas	5.779e-004	2.602e-004
o2 Gas	1.175e-005	5.291e-006
ch3 Gas	5.712e-006	2.572e-006
c2h6 Gas	8.836e-007	3.978e-007
no2 Gas	1.869e-011	8.417e-012
*c solid	1.760e+001	7.922e+000
Total Gas	2.673e+001	1.204e+001
Total Cond.	1.760e+001	7.922e+000

Reference state = reactants

H(R) = H-37.69, E(R) = E-37.68, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	18051.4	1.0243	2145.0	-125.05	-572.84	1.520	0.9559

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.072e+001	4.825e+000
n2 Gas	6.651e+000	2.995e+000
h2o Gas	5.503e+000	2.478e+000
co2 Gas	5.207e+000	2.344e+000
h2 Gas	5.153e-001	2.320e-001
ch4 Gas	2.927e-001	1.318e-001
h3n Gas	2.424e-002	1.091e-002
ch2o2 Gas	8.043e-003	3.621e-003
c2h4 Gas	5.197e-003	2.340e-003
ch2o Gas	2.279e-003	1.026e-003
ch3oh Gas	8.837e-004	3.979e-004
c2h6 Gas	1.599e-004	7.200e-005
ch3 Gas	6.245e-005	2.812e-005
no Gas	2.754e-006	1.240e-006
o2 Gas	2.787e-009	1.255e-009
no2 Gas	2.389e-013	1.076e-013
*c solid	1.486e+001	6.689e+000
Total Gas	2.893e+001	1.302e+001
Total Cond.	1.486e+001	6.689e+000

A9. HNS standard detonation without CO₂

Input>reject, co2

Input>composition, hns, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
hns	100.00	100.00	100.00	16969	258.76	0.000	450.24	c14h6n6o12

Heat of formation = 37.690 cal/gm
 Standard volume = 0.575 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 37.676 cal/gm

The elements and percent by mole

c	36.842
h	15.789
n	15.789
o	31.579

The average mol. wt. = 450.236 g/mol

Input>standard run, rho, 1.740000

The Newton line search was not successful.

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.574713 cc/gm, E0 = 37.676109 cal/gm

Using 118242 ATM as a lower bound for the C-J pressure

Using 295605 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 7 iterations

The C-J condition

The shock velocity = 8.37471e+003 m/s

The particle velocity = 1.99752e+003 m/s

The speed of sound = 6.37719e+003 m/s

P0 = 1 atm, V0 = 0.57471 cc/gm, E0 = 37.67611 cal/gm

Reference state = reactants

H(R) = H-37.69, E(R) = E-37.68, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	287272.9	0.4376	3325.9	3521.53	476.85	1.473	0.4034

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.969e+001	8.864e+000
n2 Gas	6.652e+000	2.995e+000
h2o Gas	6.613e+000	2.978e+000
o2 Gas	1.143e-001	5.148e-002
ch2o2 Gas	4.979e-002	2.242e-002

no	Gas	2.264e-002	1.019e-002
h2	Gas	8.570e-007	3.858e-007
ch3oh	Gas	2.754e-007	1.240e-007
ch2o	Gas	2.349e-007	1.058e-007
ch4	Gas	6.425e-008	2.893e-008
h3n	Gas	2.674e-008	1.204e-008
c2h4	Gas	2.103e-008	9.469e-009
no2	Gas	2.081e-012	9.369e-013
ch3	Gas	1.224e-013	5.512e-014
c2h6	Gas	7.489e-018	3.372e-018
*c	solid	1.136e+001	5.113e+000
Total Gas		3.314e+001	1.492e+001
Total Cond.		1.136e+001	5.113e+000

The C-J Adiabatic

Reference state = reactants

H(R) = H-37.69, E(R) = E-37.68, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	109839.8	0.5747	2565.8	1401.98	-126.80	1.473	0.5296

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co	Gas	1.995e+001 8.983e+000
n2	Gas	6.663e+000 3.000e+000
h2o	Gas	6.624e+000 2.982e+000
ch2o2	Gas	3.864e-002 1.740e-002
no	Gas	4.030e-004 1.815e-004
h2	Gas	2.198e-004 9.898e-005
o2	Gas	5.806e-005 2.614e-005
ch4	Gas	2.767e-005 1.246e-005
ch2o	Gas	1.495e-005 6.733e-006
h3n	Gas	7.963e-006 3.585e-006
ch3oh	Gas	7.134e-006 3.212e-006
c2h4	Gas	1.769e-006 7.966e-007
ch3	Gas	4.586e-010 2.065e-010
c2h6	Gas	2.533e-012 1.141e-012
no2	Gas	1.590e-012 7.158e-013
*c	solid	1.111e+001 5.000e+000
Total Gas		3.328e+001 1.498e+001
Total Cond.		1.111e+001 5.000e+000

Reference state = reactants

H(R) = H-37.69, E(R) = E-37.68, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	55554.1	0.6984	2145.0	577.58	-362.10	1.473	0.6499

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co	Gas	1.996e+001 8.989e+000
n2	Gas	6.663e+000 3.000e+000
h2o	Gas	6.632e+000 2.986e+000

ch2o2	Gas	2.812e-002	1.266e-002
h2	Gas	2.213e-003	9.962e-004
ch4	Gas	2.955e-004	1.330e-004
h3n	Gas	7.264e-005	3.270e-005
ch2o	Gas	6.365e-005	2.866e-005
no	Gas	2.267e-005	1.021e-005
ch3oh	Gas	1.648e-005	7.419e-006
c2h4	Gas	5.093e-006	2.293e-006
o2	Gas	4.861e-007	2.189e-007
ch3	Gas	7.075e-009	3.186e-009
c2h6	Gas	3.837e-010	1.728e-010
no2	Gas	3.279e-013	1.476e-013
*c	solid	1.110e+001	4.999e+000
Total	Gas	3.329e+001	1.499e+001
Total	Cond.	1.110e+001	4.999e+000

A10. PYX standard detonation

```

Product library title: bkwc
Executing library command: gas eos, bkwc
Executing library command: set, bkwc, alpha, 0.499123809964
Executing library command: set, bkwc, beta, 0.402655787895
Executing library command: set, bkwc, theta, 5441.84607543
Executing library command: set, bkwc, kappa, 10.8636743138
Reactant library title:# Version 2.0 by P. Clark Souers

```

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
pyx	100.00	100.00	100.00	19120	351.02	0.000	621.31	c17h7n11o16

```

Heat of formation = 30.774 cal/gm
Standard volume = 0.565 cc/gm
Standard entropy = 0.000 cal/k/gm
Standard energy = 30.761 cal/gm

```

The elements and percent by mole

c	33.333
h	13.725
n	21.569
o	31.373

The average mol. wt. = 621.314 g/mol

Input>standard run, rho, 1.770000

The Newton line search was not successful.

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.564972 cc/gm, E0 = 30.760546 cal/gm

Using 108843 ATM as a lower bound for the C-J pressure

Using 272109 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 7.51919e+003 m/s

The particle velocity = 1.88480e+003 m/s

The speed of sound = 5.63439e+003 m/s

P0 = 1 atm, V0 = 0.56497 cc/gm, E0 = 30.76055 cal/gm

Reference state = reactants

H(R) = H-30.77, E(R) = E-30.76, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	247568.0	0.4234	4004.0	2962.79	424.55	1.493	0.3705

Product concentrations

Name (mol/kg) (mol gas/mol explosive)

co2	Gas	8.882e+000	5.519e+000
n2	Gas	8.849e+000	5.498e+000
h2o	Gas	5.613e+000	3.488e+000
co	Gas	2.336e+000	1.452e+000
ch2o2	Gas	1.556e-002	9.666e-003
no	Gas	5.585e-003	3.470e-003
ch4	Gas	9.482e-004	5.892e-004
c2h4	Gas	6.602e-004	4.102e-004
o2	Gas	6.430e-004	3.995e-004
h2	Gas	5.487e-004	3.409e-004
ch3oh	Gas	2.269e-004	1.409e-004
h3n	Gas	1.392e-004	8.648e-005
ch2o	Gas	2.151e-005	1.337e-005
ch3	Gas	2.325e-008	1.445e-008
c2h6	Gas	5.732e-010	3.562e-010
no2	Gas	5.979e-012	3.715e-012
*c	solid	1.612e+001	1.002e+001
Total Gas		2.571e+001	1.597e+001
Total Cond.		1.612e+001	1.002e+001

The C-J Adiabatic

Reference state = reactants

H(R) = H-30.77, E(R) = E-30.76, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	100972.2	0.5650	3142.9	1255.31	-126.23	1.493	0.5055

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)	
n2	Gas	8.851e+000	5.499e+000
co2	Gas	7.210e+000	4.479e+000
co	Gas	5.729e+000	3.560e+000
h2o	Gas	5.567e+000	3.459e+000
ch2o2	Gas	1.751e-002	1.088e-002
h2	Gas	1.437e-002	8.926e-003
ch4	Gas	1.264e-002	7.851e-003
c2h4	Gas	2.423e-003	1.506e-003
h3n	Gas	1.889e-003	1.174e-003
ch3oh	Gas	6.313e-004	3.923e-004
no	Gas	5.632e-004	3.500e-004
ch2o	Gas	3.073e-004	1.909e-004
o2	Gas	1.053e-005	6.543e-006
ch3	Gas	1.905e-006	1.184e-006
c2h6	Gas	2.313e-007	1.437e-007
no2	Gas	1.085e-011	6.741e-012
*c	solid	1.439e+001	8.939e+000
Total Gas		2.741e+001	1.703e+001
Total Cond.		1.439e+001	8.939e+000

Reference state = reactants

H(R) = H-30.77, E(R) = E-30.76, S(R) = S- 0.00

P	V	T	H(R)	E(R)	S(R)	VGS
---	---	---	------	------	------	-----

	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	22088.9	0.9426	2145.0	-59.52	-563.75	1.493	0.8860

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	8.971e+000	5.574e+000
n2 Gas	8.844e+000	5.495e+000
co2 Gas	5.875e+000	3.650e+000
h2o Gas	5.015e+000	3.116e+000
h2 Gas	2.776e-001	1.725e-001
ch4 Gas	1.505e-001	9.348e-002
h3n Gas	1.627e-002	1.011e-002
ch2o2 Gas	7.212e-003	4.481e-003
c2h4 Gas	2.644e-003	1.643e-003
ch2o Gas	1.328e-003	8.249e-004
ch3oh Gas	5.589e-004	3.472e-004
c2h6 Gas	4.581e-005	2.846e-005
ch3 Gas	2.330e-005	1.447e-005
no Gas	3.365e-006	2.091e-006
o2 Gas	3.494e-009	2.171e-009
no2 Gas	2.069e-013	1.286e-013
*c solid	1.235e+001	7.674e+000
Total Gas	2.916e+001	1.812e+001
Total Cond.	1.235e+001	7.674e+000

A11. PYX standard detonation without CO₂

Input>reject, co2

Input>composition, pyx, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
pyx	100.00	100.00	100.00	19120	351.02	0.000	621.31	c17h7n11o16

Heat of formation = 30.774 cal/gm
 Standard volume = 0.565 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = 30.761 cal/gm

The elements and percent by mole

c	33.333
h	13.725
n	21.569
o	31.373

The average mol. wt. = 621.314 g/mol

Input>standard run, rho, 1.770000

The Newton line search was not successful.

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.564972 cc/gm, E0 = 30.760546 cal/gm

Using 128071 ATM as a lower bound for the C-J pressure

Using 320177 ATM as an upper bound for the C-J pressure

The initial P bracket of : 1.280710e+005, 3.201774e+005 did not work

The C-J function values were: 1.230534e-001, 6.407440e-003

New upper pressure limit = 420177.4

New upper pressure limit = 520177.4

The C-J point was bracketed in cjbrent

The CJ state was found in 5 iterations

The C-J condition

The shock velocity = 7.98986e+003 m/s

The particle velocity = 3.71199e+003 m/s

The speed of sound = 4.27787e+003 m/s

P0 = 1 atm, V0 = 0.56497 cc/gm, E0 = 30.76055 cal/gm

Reference state = reactants

H(R) = H-30.77, E(R) = E-30.76, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	518088.0	0.3025	3697.9	5442.06	1646.68	1.384	0.2656

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
n2 Gas	8.787e+000	5.460e+000
o2 Gas	7.673e+000	4.767e+000

h2o	Gas	5.627e+000	3.496e+000
co	Gas	4.637e+000	2.881e+000
no	Gas	1.297e-001	8.056e-002
ch2o2	Gas	6.517e-003	4.049e-003
h2	Gas	2.070e-009	1.286e-009
ch3oh	Gas	1.351e-009	8.393e-010
ch2o	Gas	3.373e-010	2.096e-010
ch4	Gas	6.061e-011	3.766e-011
h3n	Gas	5.378e-011	3.341e-011
c2h4	Gas	2.224e-011	1.382e-011
no2	Gas	2.174e-014	1.351e-014
ch3	Gas	1.926e-018	1.196e-018
c2h6	Gas	1.314e-024	8.167e-025
*c	solid	2.272e+001	1.411e+001
Total Gas		2.686e+001	1.669e+001
Total Cond.		2.272e+001	1.411e+001

The C-J Adiabatic

Reference state = reactants

H(R) = H-30.77, E(R) = E-30.76, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	108460.1	0.5650	2153.9	1238.32	-245.67	1.384	0.5356

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co	Gas	2.009e+001
n2	Gas	8.852e+000
h2o	Gas	5.604e+000
ch2o2	Gas	2.897e-002
no	Gas	9.492e-005
o2	Gas	1.710e-005
h2	Gas	1.424e-005
ch2o	Gas	1.193e-006
ch4	Gas	8.470e-007
h3n	Gas	4.119e-007
ch3oh	Gas	3.393e-007
c2h4	Gas	1.822e-008
ch3	Gas	1.533e-012
no2	Gas	6.240e-014
c2h6	Gas	3.514e-015
*c	solid	7.243e+000
Total Gas		3.458e+001
Total Cond.		7.243e+000

Reference state = reactants

H(R) = H-30.77, E(R) = E-30.76, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	107026.3	0.5669	2145.0	1218.67	-250.81	1.384	0.5375

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
------	----------	-------------------------

co	Gas	2.009e+001	1.248e+001
n2	Gas	8.852e+000	5.500e+000
h2o	Gas	5.604e+000	3.482e+000
ch2o2	Gas	2.885e-002	1.793e-002
no	Gas	8.864e-005	5.507e-005
o2	Gas	1.529e-005	9.497e-006
h2	Gas	1.499e-005	9.314e-006
ch2o	Gas	1.234e-006	7.665e-007
ch4	Gas	8.902e-007	5.531e-007
h3n	Gas	4.329e-007	2.690e-007
ch3oh	Gas	3.452e-007	2.145e-007
c2h4	Gas	1.851e-008	1.150e-008
ch3	Gas	1.626e-012	1.010e-012
no2	Gas	6.042e-014	3.754e-014
c2h6	Gas	3.929e-015	2.441e-015
*c	solid	7.243e+000	4.500e+000
Total	Gas	3.458e+001	2.148e+001
Total	Cond.	7.243e+000	4.500e+000

A12. PETN gun without CO₂

Input>reject, co2

Input>composition, petn, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm

Standard volume = 0.562 cc/gm

Standard entropy = 0.000 cal/k/gm

Standard energy = -398.425 cal/gm

The elements and percent by mole

c	17.241
h	27.586
n	13.793
o	41.379

The average mol. wt. = 316.146 g/mol

Input>gun, 0.500000, 0.250000, 1.000000

GUN calculation:

WARNING: Results will not match BLAKE -- the virial EOS is not being used

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
The initial damping was too small								
Undertaking a gradient line search instead								
The initial damping was too small								
Undertaking a gradient line search instead								
The initial damping was too small								
Undertaking a gradient line search instead								
Too many iterations in the etanewt solver								
Failed to find equilibrium. Will try again.								
The initial damping was too small								
Undertaking a gradient line search instead								
1.)	0.5000	2852.5	925.5	937.51	25.299	0.987	1.215	1.974
2.)	0.7500	2781.9	1852.1	914.12	25.304	0.840	1.221	2.701
3.)	1.0000	2696.4	3231.7	885.87	25.308	0.726	1.232	3.648

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
co	Gas	1.580e+001	1.580e+001	1.579e+001
h2o	Gas	1.264e+001	1.263e+001	1.263e+001
n2	Gas	6.100e+000	6.145e+000	6.190e+000
o2	Gas	4.520e+000	4.564e+000	4.608e+000
no	Gas	4.489e-001	3.615e-001	2.726e-001
ch2o2	Gas	1.160e-002	1.885e-002	2.613e-002
h2	Gas	4.522e-003	1.245e-003	2.725e-004
no2	Gas	2.820e-003	8.911e-004	1.699e-004
ch2o	Gas	8.426e-006	4.738e-006	1.936e-006
h3n	Gas	1.869e-006	7.870e-007	2.385e-007
ch3oh	Gas	6.472e-010	6.208e-010	4.390e-010
ch4	Gas	4.533e-011	2.892e-011	1.407e-011
ch3	Gas	2.206e-011	4.636e-012	5.740e-013

c2h4	Gas	3.204e-016	3.152e-016	2.331e-016
c2h6	Gas	8.248e-021	3.205e-021	6.095e-022
*c	solid	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.953e+001	3.952e+001	3.951e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000

A13. PETN gun, confined space

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm
 Standard volume = 0.562 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -398.425 cal/gm

The elements and percent by mole

c	17.241
h	27.586
n	13.793
o	41.379

The average mol. wt. = 316.146 g/mol
 Input>gun, 0.500000, 0.250000, 1.000000

GUN calculation:

WARNING: Results will not match BLAKE -- the virial EOS is not being used

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.5000	4282.1	1182.2	1256.83	28.329	0.937	1.164	1.881
2.)	0.7500	4264.4	2333.6	1242.34	28.540	0.801	1.160	2.505
3.)	1.0000	4191.0	4006.5	1215.47	28.670	0.697	1.159	3.296

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
h2o	Gas	1.206e+001	1.227e+001	1.241e+001
co2	Gas	9.035e+000	9.335e+000	9.486e+000
co	Gas	6.771e+000	6.465e+000	6.307e+000
n2	Gas	6.113e+000	6.198e+000	6.261e+000
h2	Gas	5.776e-001	3.643e-001	2.139e-001
no	Gas	4.242e-001	2.545e-001	1.279e-001
o2	Gas	3.049e-001	1.343e-001	4.700e-002
ch2o2	Gas	8.653e-003	1.448e-002	2.111e-002
h3n	Gas	1.861e-003	2.422e-003	2.766e-003
ch2o	Gas	6.584e-004	8.087e-004	8.536e-004
no2	Gas	5.337e-004	1.090e-004	1.222e-005
ch3	Gas	3.023e-006	4.133e-006	4.710e-006
ch4	Gas	2.882e-006	1.109e-005	4.504e-005
ch3oh	Gas	2.613e-006	9.102e-006	2.906e-005
c2h4	Gas	1.382e-009	1.388e-008	1.560e-007
c2h6	Gas	1.242e-012	1.119e-011	8.998e-011

```
*c solid 0.000e+000 0.000e+000 0.000e+000

Total Gas 3.530e+001 3.504e+001 3.488e+001
Total Cond. 0.000e+000 0.000e+000 0.000e+000
Input>point, p, 100000.000000, t, 3000.000000
```

```
Reference state = reactants
H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00
```

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	100000.0	0.6048	3000.0	1097.09	-367.54	1.676	0.6048

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.253e+001	3.961e+000
co2 Gas	9.623e+000	3.042e+000
n2 Gas	6.325e+000	2.000e+000
co Gas	6.127e+000	1.937e+000
ch4 Gas	2.947e-002	9.317e-003
ch2o2 Gas	2.627e-002	8.305e-003
h2 Gas	2.188e-002	6.916e-003
c2h4 Gas	4.155e-003	1.314e-003
h3n Gas	2.539e-003	8.028e-004
ch3oh Gas	1.276e-003	4.035e-004
ch2o Gas	3.463e-004	1.095e-004
no Gas	3.348e-004	1.058e-004
o2 Gas	7.982e-006	2.523e-006
ch3 Gas	1.850e-006	5.848e-007
c2h6 Gas	4.360e-007	1.378e-007
no2 Gas	3.052e-012	9.647e-013
*c solid	1.776e-033	5.616e-034

```
Total Gas 3.469e+001 1.097e+001
Total Cond. 1.776e-033 5.616e-034
Input>explosion, rho, 1.000000
```

The Constant Volume Explosion State:

```
Reference state = reactants
H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00
```

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	39541.5	1.0000	4191.0	957.60	0.00	1.945	1.0000

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.241e+001	3.924e+000
co2 Gas	9.486e+000	2.999e+000
co Gas	6.307e+000	1.994e+000
n2 Gas	6.261e+000	1.979e+000
h2 Gas	2.139e-001	6.762e-002
no Gas	1.279e-001	4.044e-002

o2	Gas	4.700e-002	1.486e-002
ch2o2	Gas	2.111e-002	6.674e-003
h3n	Gas	2.766e-003	8.743e-004
ch2o	Gas	8.536e-004	2.699e-004
ch4	Gas	4.504e-005	1.424e-005
ch3oh	Gas	2.906e-005	9.188e-006
no2	Gas	1.222e-005	3.863e-006
ch3	Gas	4.710e-006	1.489e-006
c2h4	Gas	1.560e-007	4.930e-008
c2h6	Gas	8.998e-011	2.845e-011
*c	solid	0.000e+000	0.000e+000
Total	Gas	3.488e+001	1.103e+001
Total	Cond.	0.000e+000	0.000e+000

A14. PETN gun, confined space, without CO₂ byproduct

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm
 Standard volume = 0.562 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -398.425 cal/gm

The elements and percent by mole

c	17.241
h	27.586
n	13.793
o	41.379

The average mol. wt. = 316.146 g/mol

Input>reject, co2

Input>composition, petn, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm
 Standard volume = 0.562 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -398.425 cal/gm

The elements and percent by mole

c	17.241
h	27.586
n	13.793
o	41.379

The average mol. wt. = 316.146 g/mol

Input>gun, 0.500000, 0.250000, 1.000000

GUN calculation:

WARNING: Results will not match BLAKE -- the virial EOS is not being used

Rho	Temp	Pressure	Impetus	Mol Wt.	Covol	Frozen	Phi
g/cc	K	MPa	J/g	Gas	cc/g	Cp/Cv	
The initial damping was too small							
Undertaking a gradient line search instead							

The initial damping was too small
 Undertaking a gradient line search instead
 The initial damping was too small
 Undertaking a gradient line search instead
 Too many iterations in the etanewt solver
 Failed to find equilibrium. Will try again.
 The initial damping was too small
 Undertaking a gradient line search instead
 1.) 0.5000 2852.5 925.5 937.51 25.299 0.987 1.215 1.974
 2.) 0.7500 2781.9 1852.1 914.12 25.304 0.840 1.221 2.701
 3.) 1.0000 2696.4 3231.7 885.87 25.308 0.726 1.232 3.648

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
co	Gas	1.580e+001	1.580e+001	1.579e+001
h2o	Gas	1.264e+001	1.263e+001	1.263e+001
n2	Gas	6.100e+000	6.145e+000	6.190e+000
o2	Gas	4.520e+000	4.564e+000	4.608e+000
no	Gas	4.489e-001	3.615e-001	2.726e-001
ch2o2	Gas	1.160e-002	1.885e-002	2.613e-002
h2	Gas	4.522e-003	1.245e-003	2.725e-004
no2	Gas	2.820e-003	8.911e-004	1.699e-004
ch2o	Gas	8.426e-006	4.738e-006	1.936e-006
h3n	Gas	1.869e-006	7.870e-007	2.385e-007
ch3oh	Gas	6.472e-010	6.208e-010	4.390e-010
ch4	Gas	4.533e-011	2.892e-011	1.407e-011
ch3	Gas	2.206e-011	4.636e-012	5.740e-013
c2h4	Gas	3.204e-016	3.152e-016	2.331e-016
c2h6	Gas	8.248e-021	3.205e-021	6.095e-022
*c	solid	0.000e+000	0.000e+000	0.000e+000
Total Gas		3.953e+001	3.952e+001	3.951e+001
Total Cond.		0.000e+000	0.000e+000	0.000e+000

Input>point, p, 100000.000000, t, 3000.000000

The Constant Volume Explosion State:

Reference state = reactants
 $H(R) = H - 398.41$, $E(R) = E - 398.42$, $S(R) = S - 0.00$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	31894.2	1.0000	2696.4	772.40	-0.00	1.850	1.0000

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.579e+001	4.992e+000
h2o Gas	1.263e+001	3.992e+000
n2 Gas	6.190e+000	1.957e+000
o2 Gas	4.608e+000	1.457e+000
no Gas	2.726e-001	8.618e-002
ch2o2 Gas	2.613e-002	8.260e-003
h2 Gas	2.725e-004	8.616e-005
no2 Gas	1.699e-004	5.372e-005
ch2o Gas	1.936e-006	6.120e-007
h3n Gas	2.385e-007	7.539e-008
ch3oh Gas	4.390e-010	1.388e-010

ch4	Gas	1.407e-011	4.448e-012
ch3	Gas	5.740e-013	1.815e-013
c2h4	Gas	2.331e-016	7.368e-017
c2h6	Gas	6.095e-022	1.927e-022
*c	solid	0.000e+000	0.000e+000
Total	Gas	3.951e+001	1.249e+001
Total	Cond.	0.000e+000	0.000e+000

A15. PETN standard detonation

Product library title: bkwc
 Executing library command: gas eos, bkw
 Executing library command: set, bkw, alpha, 0.499123809964
 Executing library command: set, bkw, beta, 0.402655787895
 Executing library command: set, bkw, theta, 5441.84607543
 Executing library command: set, bkw, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm
 Standard volume = 0.562 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -398.425 cal/gm

The elements and percent by mole

c	17.241
h	27.586
n	13.793
o	41.379

The average mol. wt. = 316.146 g/mol

Input>standard run, rho, 1.778000

The initial damping was too small

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The initial damping was too small

Undertaking a gradient line search instead

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.562430 cc/gm, E0 = -398.424554 cal/gm

Using 140542 ATM as a lower bound for the C-J pressure

Using 351354 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 8.57597e+003 m/s

The particle velocity = 2.06721e+003 m/s

The speed of sound = 6.50876e+003 m/s

P0 = 1 atm, V0 = 0.56243 cc/gm, E0 = -398.42455 cal/gm

Reference state = reactants

H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	311088.7	0.4269	4351.7	3726.61	510.70	1.704	0.4212

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.262e+001 3.991e+000
co2	Gas	1.144e+001 3.618e+000
n2	Gas	6.321e+000 1.998e+000
co	Gas	2.382e+000 7.532e-001
ch2o2	Gas	2.355e-002 7.445e-003
no	Gas	1.074e-002 3.396e-003
o2	Gas	3.070e-003 9.707e-004
ch4	Gas	1.235e-003 3.906e-004
c2h4	Gas	1.109e-003 3.506e-004
h2	Gas	4.699e-004 1.486e-004
ch3oh	Gas	4.089e-004 1.293e-004
h3n	Gas	1.056e-004 3.339e-005
ch2o	Gas	1.591e-005 5.028e-006
ch3	Gas	1.269e-008 4.011e-009
c2h6	Gas	2.690e-010 8.503e-011
no2	Gas	3.299e-012 1.043e-012
*c	solid	1.962e+000 6.202e-001
Total Gas		3.281e+001 1.037e+001
Total Cond.		1.962e+000 6.202e-001

The C-J Adiabatic

Reference state = reactants

$$H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00$$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	131718.4	0.5624	3372.1	1634.01	-160.11	1.704	0.5623

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.255e+001 3.967e+000
co2	Gas	9.617e+000 3.040e+000
n2	Gas	6.325e+000 2.000e+000
co	Gas	6.107e+000 1.931e+000
ch2o2	Gas	3.264e-002 1.032e-002
ch4	Gas	2.072e-002 6.549e-003
h2	Gas	1.334e-002 4.218e-003
c2h4	Gas	5.612e-003 1.774e-003
h3n	Gas	1.754e-003 5.545e-004
ch3oh	Gas	1.514e-003 4.788e-004
no	Gas	1.134e-003 3.586e-004
ch2o	Gas	2.956e-004 9.345e-005
o2	Gas	5.065e-005 1.601e-005
ch3	Gas	1.491e-006 4.715e-007
c2h6	Gas	1.954e-007 6.178e-008
no2	Gas	8.392e-012 2.653e-012
*c	solid	2.521e-002 7.970e-003
Total Gas		3.467e+001 1.096e+001
Total Cond.		2.521e-002 7.970e-003

Reference state = reactants

$$H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00$$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	17236.5	1.1483	2145.0	-361.00	-840.33	1.704	1.1483

Product concentrations

Name		(mol/kg)	(mol gas/mol explosive)
h2o	Gas	1.226e+001	3.876e+000
co2	Gas	9.884e+000	3.125e+000
n2	Gas	6.321e+000	1.998e+000
co	Gas	5.912e+000	1.869e+000
h2	Gas	3.450e-001	1.091e-001
ch4	Gas	1.133e-002	3.581e-003
h3n	Gas	9.696e-003	3.065e-003
ch2o2	Gas	7.653e-003	2.419e-003
ch2o	Gas	6.425e-004	2.031e-004
ch3oh	Gas	1.193e-004	3.771e-005
c2h4	Gas	2.386e-005	7.542e-006
no	Gas	1.075e-005	3.400e-006
ch3	Gas	3.640e-006	1.151e-006
c2h6	Gas	3.872e-007	1.224e-007
o2	Gas	4.398e-008	1.390e-008
no2	Gas	3.529e-012	1.116e-012
*c	solid	0.000e+000	0.000e+000
Total	Gas	3.475e+001	1.099e+001
Total	Cond.	0.000e+000	0.000e+000

A16. PETN standard detonation without CO₂ byproduct

Input>reject, co2

Input>composition, petn, 100, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm

Standard volume = 0.562 cc/gm

Standard entropy = 0.000 cal/k/gm

Standard energy = -398.425 cal/gm

The elements and percent by mole

c 17.241

h 27.586

n 13.793

o 41.379

The average mol. wt. = 316.146 g/mol

Input>standard run, rho, 1.778000

The Newton line search was not successful.

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.562430 cc/gm, E0 = -398.424554 cal/gm

Using 118404 ATM as a lower bound for the C-J pressure

Using 296011 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 8.55883e+003 m/s

The particle velocity = 1.73543e+003 m/s

The speed of sound = 6.82340e+003 m/s

P0 = 1 atm, V0 = 0.56243 cc/gm, E0 = -398.42455 cal/gm

Reference state = reactants

H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P (ATM)	V (CC/GM)	T (K)	H(R) (CAL/GM)	E(R) (CAL/GM)	S(R) (CAL/K/GM)	VGS (CC/GM)
1.)	260638.0	0.4484	2754.0	3190.20	359.92	1.545	0.4484

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.579e+001	4.991e+000

h2o	Gas	1.262e+001	3.991e+000
n2	Gas	6.298e+000	1.991e+000
o2	Gas	4.716e+000	1.491e+000
no	Gas	5.690e-002	1.799e-002
ch2o2	Gas	2.821e-002	8.920e-003
h2	Gas	1.493e-008	4.719e-009
ch2o	Gas	1.962e-009	6.201e-010
ch3oh	Gas	2.742e-010	8.669e-011
h3n	Gas	8.796e-011	2.781e-011
ch4	Gas	6.252e-012	1.977e-012
no2	Gas	3.258e-012	1.030e-012
c2h4	Gas	5.542e-014	1.752e-014
ch3	Gas	2.668e-018	8.434e-019
c2h6	Gas	2.183e-025	6.901e-026
*c	solid	0.000e+000	0.000e+000
Total Gas		3.951e+001	1.249e+001
Total Cond.		0.000e+000	0.000e+000

The C-J Adiabatic

Reference state = reactants

H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	118947.1	0.5495	2145.0	1507.50	-75.38	1.545	0.5495

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co	Gas	1.579e+001 4.991e+000
h2o	Gas	1.262e+001 3.991e+000
n2	Gas	6.308e+000 1.994e+000
o2	Gas	4.727e+000 1.494e+000
no	Gas	3.574e-002 1.130e-002
ch2o2	Gas	2.956e-002 9.345e-003
h2	Gas	3.212e-008 1.015e-008
no2	Gas	2.359e-009 7.458e-010
ch2o	Gas	1.558e-009 4.926e-010
h3n	Gas	3.888e-011 1.229e-011
ch3oh	Gas	2.371e-012 7.495e-013
ch4	Gas	1.393e-014 4.404e-015
c2h4	Gas	5.388e-019 1.704e-019
ch3	Gas	1.602e-019 5.065e-020
c2h6	Gas	1.027e-028 3.247e-029
*c	solid	0.000e+000 0.000e+000
Total Gas		3.951e+001 1.249e+001
Total Cond.		0.000e+000 0.000e+000

Reference state = reactants

H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	108962.3	0.5624	2085.5	1373.09	-111.06	1.545	0.5624

Product concentrations

	Name	(mol/kg)	(mol gas/mol explosive)
*	co Gas	1.579e+001	4.991e+000
*	h2o Gas	1.262e+001	3.991e+000
*	n2 Gas	6.308e+000	1.994e+000
*	o2 Gas	4.727e+000	1.494e+000
*	no Gas	3.574e-002	1.130e-002
*	ch2o2 Gas	2.956e-002	9.345e-003
*	h2 Gas	3.212e-008	1.015e-008
*	no2 Gas	2.359e-009	7.458e-010
*	ch2o Gas	1.558e-009	4.926e-010
*	h3n Gas	3.888e-011	1.229e-011
*	ch3oh Gas	2.371e-012	7.495e-013
*	ch4 Gas	1.393e-014	4.404e-015
*	c2h4 Gas	5.388e-019	1.704e-019
*	ch3 Gas	1.602e-019	5.065e-020
*	c2h6 Gas	1.027e-028	3.247e-029
*	*c solid	0.000e+000	0.000e+000
	Total Gas	3.951e+001	1.249e+001
	Total Cond.	0.000e+000	0.000e+000

A17. PETN standard detonation, confined space

Product library title: bkwc
 Executing library command: gas eos, bkwc
 Executing library command: set, bkwc, alpha, 0.499123809964
 Executing library command: set, bkwc, beta, 0.402655787895
 Executing library command: set, bkwc, theta, 5441.84607543
 Executing library command: set, bkwc, kappa, 10.8636743138
 Reactant library title:# Version 2.0 by P. Clark Souers

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.81	0.000	316.15	c5h8n4o12

Heat of formation = -398.411 cal/gm
 Standard volume = 0.562 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -398.425 cal/gm

The elements and percent by mole

c	17.241
h	27.586
n	13.793
o	41.379

The average mol. wt. = 316.146 g/mol

Input>standard run, rho, 1.778000

The initial damping was too small

Undertaking a gradient line search instead

The initial damping was too small

Undertaking a gradient line search instead

Too many iterations in the etanewt solver

Failed to find equilibrium. Will try again.

The initial damping was too small

Undertaking a gradient line search instead

The hugoniot reference state:

P0 = 1.000000 ATM, V0 = 0.562430 cc/gm, E0 = -398.424554 cal/gm

Using 140542 ATM as a lower bound for the C-J pressure

Using 351354 ATM as an upper bound for the C-J pressure

The C-J point was bracketed in cjbrent

The CJ state was found in 6 iterations

The C-J condition

The shock velocity = 8.57597e+003 m/s

The particle velocity = 2.06721e+003 m/s

The speed of sound = 6.50876e+003 m/s

P0 = 1 atm, V0 = 0.56243 cc/gm, E0 = -398.42455 cal/gm

Reference state = reactants

H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

P	V	T	H(R)	E(R)	S(R)	VGS
(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)

1.) 311088.7 0.4269 4351.7 3726.61 510.70 1.704 0.4212

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.262e+001	3.991e+000
co2 Gas	1.144e+001	3.618e+000
n2 Gas	6.321e+000	1.998e+000
co Gas	2.382e+000	7.532e-001
ch2o2 Gas	2.355e-002	7.445e-003
no Gas	1.074e-002	3.396e-003
o2 Gas	3.070e-003	9.707e-004
ch4 Gas	1.235e-003	3.906e-004
c2h4 Gas	1.109e-003	3.506e-004
h2 Gas	4.699e-004	1.486e-004
ch3oh Gas	4.089e-004	1.293e-004
h3n Gas	1.056e-004	3.339e-005
ch2o Gas	1.591e-005	5.028e-006
ch3 Gas	1.269e-008	4.011e-009
c2h6 Gas	2.690e-010	8.503e-011
no2 Gas	3.299e-012	1.043e-012
*c solid	1.962e+000	6.202e-001
Total Gas	3.281e+001	1.037e+001
Total Cond.	1.962e+000	6.202e-001

The C-J Adiabatic

Reference state = reactants

H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

P	V	T	H(R)	E(R)	S(R)	VGS
(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.) 17236.5	1.1483	2145.0	-361.00	-840.33	1.704	1.1483

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.226e+001	3.876e+000
co2 Gas	9.884e+000	3.125e+000
n2 Gas	6.321e+000	1.998e+000
co Gas	5.912e+000	1.869e+000
h2 Gas	3.450e-001	1.091e-001
ch4 Gas	1.133e-002	3.581e-003
h3n Gas	9.696e-003	3.065e-003
ch2o2 Gas	7.653e-003	2.419e-003
ch2o Gas	6.425e-004	2.031e-004
ch3oh Gas	1.193e-004	3.771e-005
c2h4 Gas	2.386e-005	7.542e-006
no Gas	1.075e-005	3.400e-006
ch3 Gas	3.640e-006	1.151e-006
c2h6 Gas	3.872e-007	1.224e-007
o2 Gas	4.398e-008	1.390e-008
no2 Gas	3.529e-012	1.116e-012
*c solid	0.000e+000	0.000e+000
Total Gas	3.475e+001	1.099e+001
Total Cond.	0.000e+000	0.000e+000

The Constant Volume Explosion State:

Reference state = reactants
 H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	39541.5	1.0000	4191.0	957.60	0.00	1.945	1.0000

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
h2o Gas	1.241e+001	3.924e+000
co2 Gas	9.486e+000	2.999e+000
co Gas	6.307e+000	1.994e+000
n2 Gas	6.261e+000	1.979e+000
h2 Gas	2.139e-001	6.762e-002
no Gas	1.279e-001	4.044e-002
o2 Gas	4.700e-002	1.486e-002
ch2o2 Gas	2.111e-002	6.674e-003
h3n Gas	2.766e-003	8.743e-004
ch2o Gas	8.536e-004	2.699e-004
ch4 Gas	4.504e-005	1.424e-005
ch3oh Gas	2.906e-005	9.188e-006
no2 Gas	1.222e-005	3.863e-006
ch3 Gas	4.710e-006	1.489e-006
Total Gas	3.488e+001	1.103e+001
Total Cond.	0.000e+000	0.000e+000

A18. PETN standard detonation, confined space without CO₂ byproduct

Input>standard run, rho, 1.778000
 The hugoniot reference state:
 P0 = 1.000000 ATM, V0 = 0.562430 cc/gm, E0 = -398.424554 cal/gm
 Using 118404 ATM as a lower bound for the C-J pressure
 Using 296011 ATM as an upper bound for the C-J pressure
 The C-J point was bracketed in cjbrent
 The CJ state was found in 6 iterations
 The C-J condition

The shock velocity = 8.55883e+003 m/s
 The particle velocity = 1.73543e+003 m/s
 The speed of sound = 6.82340e+003 m/s

P0 = 1 atm, V0 = 0.56243 cc/gm, E0 = -398.42455 cal/gm

Reference state = reactants
 H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	260638.0	0.4484	2754.0	3190.20	359.92	1.545	0.4484

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.579e+001	4.991e+000
h2o Gas	1.262e+001	3.991e+000
n2 Gas	6.298e+000	1.991e+000
o2 Gas	4.716e+000	1.491e+000
no Gas	5.690e-002	1.799e-002
ch2o2 Gas	2.821e-002	8.920e-003
h2 Gas	1.493e-008	4.719e-009
ch2o Gas	1.962e-009	6.201e-010
ch3oh Gas	2.742e-010	8.669e-011
h3n Gas	8.796e-011	2.781e-011
ch4 Gas	6.252e-012	1.977e-012
no2 Gas	3.258e-012	1.030e-012
c2h4 Gas	5.542e-014	1.752e-014
ch3 Gas	2.668e-018	8.434e-019
c2h6 Gas	2.183e-025	6.901e-026
*c solid	0.000e+000	0.000e+000
Total Gas	3.951e+001	1.249e+001
Total Cond.	0.000e+000	0.000e+000

The C-J Adiabatic

Reference state = reactants
 H(R) = H--398.41, E(R) = E--398.42, S(R) = S- 0.00

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	118947.1	0.5495	2145.0	1507.50	-75.38	1.545	0.5495

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.579e+001	4.991e+000
h2o Gas	1.262e+001	3.991e+000
n2 Gas	6.308e+000	1.994e+000
o2 Gas	4.727e+000	1.494e+000
no Gas	3.574e-002	1.130e-002
ch2o2 Gas	2.956e-002	9.345e-003
h2 Gas	3.212e-008	1.015e-008
no2 Gas	2.359e-009	7.458e-010
ch2o Gas	1.558e-009	4.926e-010
h3n Gas	3.888e-011	1.229e-011
ch3oh Gas	2.371e-012	7.495e-013
ch4 Gas	1.393e-014	4.404e-015
c2h4 Gas	5.388e-019	1.704e-019
ch3 Gas	1.602e-019	5.065e-020
c2h6 Gas	1.027e-028	3.247e-029
*c solid	0.000e+000	0.000e+000
Total Gas	3.951e+001	1.249e+001
Total Cond.	0.000e+000	0.000e+000

Input>explosion, rho, 1.000000

The Constant Volume Explosion State:

Reference state = reactants
 $H(R) = H - 398.41$, $E(R) = E - 398.42$, $S(R) = S - 0.00$

	P	V	T	H(R)	E(R)	S(R)	VGS
	(ATM)	(CC/GM)	(K)	(CAL/GM)	(CAL/GM)	(CAL/K/GM)	(CC/GM)
1.)	31894.2	1.0000	2696.4	772.40	-0.00	1.850	1.0000

Product concentrations

Name	(mol/kg)	(mol gas/mol explosive)
co Gas	1.579e+001	4.992e+000
h2o Gas	1.263e+001	3.992e+000
n2 Gas	6.190e+000	1.957e+000
o2 Gas	4.608e+000	1.457e+000
no Gas	2.726e-001	8.618e-002
ch2o2 Gas	2.613e-002	8.260e-003
h2 Gas	2.725e-004	8.616e-005
no2 Gas	1.699e-004	5.372e-005
ch2o Gas	1.936e-006	6.120e-007
h3n Gas	2.385e-007	7.539e-008
ch3oh Gas	4.390e-010	1.388e-010
ch4 Gas	1.407e-011	4.448e-012
ch3 Gas	5.740e-013	1.815e-013
c2h4 Gas	2.331e-016	7.368e-017
c2h6 Gas	6.095e-022	1.927e-022
*c solid	0.000e+000	0.000e+000
Total Gas	3.951e+001	1.249e+001
Total Cond.	0.000e+000	0.000e+000

Appendix B

Ambient Modeling Results, Unit Concentrations

Appendix B

Ambient Modeling Results, Unit Concentrations

Offshore modeling, OCD5

Table B-1. Vertical Discharge, without a surrounding building

Table B-2. Vertical Discharge, with a nearby building

Table B-3. Horizontal Discharge, without a surrounding building

Table B-4. Horizontal Discharge, with a nearby building

Onshore Modeling, ISC-Prime

Table B-5. Vertical Discharge, without a surrounding building

Table B-6. Horizontal Discharge, with a nearby building

Table B-1. Offshore 1hr Conc - Source and Receptors are on Platform, 1994 (Vertical discharge Without a Surrounding Building)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour		ug/m3	ppm
1	23.78	27.14	5	10	4759.75	279	11	Max Conc at 5m:	4761.7	4.16
2	23.78	27.14	5	20	4755.08	10	13	Max Conc at 10m:	11218.0	9.80
3	23.78	27.14	5	30	4748.89	122	23	Max Conc at 20m:	7557.8	6.60
4	23.78	27.14	5	40	4752.88	163	12	Max Conc at 30m:	6269.6	5.47
5	23.78	27.14	5	50	4760.56	64	21			
6	23.78	27.14	5	60	4761.66	3	4	Avg Conc at 5m:	4753.9	4.15
7	23.78	27.14	5	70	4761.33	132	10	Avg Conc at 10m:	11210.4	9.79
8	23.78	27.14	5	80	4758.6	140	12	Avg Conc at 20m:	7493.5	6.54
9	23.78	27.14	5	90	4760.04	222	18	Avg Conc at 30m:	5837.9	5.10
10	23.78	27.14	5	100	4758.6	18	8			
11	23.78	27.14	5	110	4761.33	325	8	St Dev of Conc at 5m:	47.8	0.01
12	23.78	27.14	5	120	4761.66	118	3	St Dev of Conc at 10m:	182.3	0.01
13	23.78	27.14	5	130	4753.29	181	13	St Dev of Conc at 20m:	5306.4	0.06
14	23.78	27.14	5	140	4759.75	17	15	St Dev of Conc at 30m:	54125.6	0.20
15	23.78	27.13	5	150	4755.9	310	14			
16	23.78	27.13	5	160	4755.09	300	17			
17	23.78	27.13	5	170	4759.75	197	8			
18	23.78	27.13	5	180	4753.39	54	12			
19	23.78	27.13	5	190	4758.6	33	11			
20	23.77	27.13	5	200	4745.77	2	12			
21	23.77	27.13	5	210	4752.58	17	9			
22	23.77	27.14	5	220	4748.34	45	12			
23	23.77	27.14	5	230	4755.47	300	15			
24	23.77	27.14	5	240	4755.9	190	15			
25	23.77	27.14	5	250	4755.09	325	7			
26	23.77	27.14	5	260	4744.93	261	19			
27	23.77	27.14	5	270	4753.39	144	18			
28	23.77	27.14	5	280	4744.88	350	10			

(continued)

Table B-1. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3	ppm
28	23.77	27.14	5	280	4744.88	350	10		
29	23.77	27.14	5	290	4748.1	62	20		
30	23.77	27.14	5	300	4755.89	337	13		
31	23.77	27.14	5	310	4748.36	86	19		
32	23.77	27.14	5	320	4726.89	263	13		
33	23.77	27.14	5	330	4752.58	106	13		
34	23.77	27.14	5	340	4745.82	63	6		
35	23.78	27.14	5	350	4758.6	333	4		
36	23.78	27.14	5	360	4753.39	129	18		
37	23.78	27.15	10	10	11217.35	279	11		
38	23.78	27.15	10	20	11216.74	10	13		
39	23.78	27.15	10	30	11200	122	23		
40	23.78	27.15	10	40	11199.65	163	12		
41	23.78	27.15	10	50	11216.78	64	21		
42	23.78	27.14	10	60	11217.04	3	4		
43	23.79	27.14	10	70	11217.05	132	10		
44	23.79	27.14	10	80	11216.66	140	12		
45	23.79	27.14	10	90	11217.14	222	18		
46	23.79	27.14	10	100	11216.66	18	8		
47	23.79	27.14	10	110	11217.03	325	8		
48	23.78	27.13	10	120	11217.02	118	3		
49	23.78	27.13	10	130	11199.06	181	13		
50	23.78	27.13	10	140	11216.91	17	15		
51	23.78	27.13	10	150	11217.35	310	14		
52	23.78	27.13	10	160	11216.76	300	17		
53	23.78	27.13	10	170	11217.35	197	8		
54	23.78	27.13	10	180	11217.14	54	12		
55	23.77	27.13	10	190	11217.5	33	11		
56	23.77	27.13	10	200	11199.4	2	12		
57	23.77	27.13	10	210	11217.77	17	9		

(continued)

Table B-1. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3	ppm
58	23.77	27.13	10	220	11199.79	45	12		
59	23.77	27.13	10	230	11217.44	300	15		
60	23.77	27.13	10	240	11217.77	190	15		
61	23.77	27.14	10	250	11217.85	325	7		
62	23.77	27.14	10	260	11199.94	261	19		
63	23.77	27.14	10	270	11217.99	144	18		
64	23.77	27.14	10	280	11199.67	350	10		
65	23.77	27.14	10	290	11200.21	62	20		
66	23.77	27.14	10	300	11217.76	337	13		
67	23.77	27.15	10	310	11199.85	86	19		
68	23.77	27.15	10	320	11146.72	263	13		
69	23.77	27.15	10	330	11217.77	106	13		
70	23.77	27.15	10	340	11199.5	63	6		
71	23.77	27.15	10	350	11217.5	333	4		
72	23.78	27.15	10	360	11217.14	129	18		
73	23.78	27.16	20	10	7557.69	260	6		
74	23.78	27.16	20	20	7557.59	183	9		
75	23.79	27.16	20	30	7552.29	93	13		
76	23.79	27.15	20	40	7557.19	133	9		
77	23.79	27.15	20	50	7493.19	213	14		
78	23.79	27.15	20	60	7536.65	165	1		
79	23.79	27.15	20	70	7534.99	195	14		
80	23.8	27.14	20	80	7541.6	91	21		
81	23.8	27.14	20	90	7557.44	347	11		
82	23.8	27.14	20	100	7557.27	20	21		
83	23.79	27.13	20	110	7556.89	163	19		
84	23.79	27.13	20	120	7492.46	22	11		
85	23.79	27.13	20	130	7483.84	11	1		
86	23.79	27.12	20	140	7356.01	228	6		
87	23.79	27.12	20	150	7290.36	44	13		

(continued)

Table B-1. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3	ppm
88	23.78	27.12	20	160	7297.43	109	21		
89	23.78	27.12	20	170	7529.26	58	9		
90	23.78	27.12	20	180	7554.05	58	10		
91	23.77	27.12	20	190	7470.91	201	9		
92	23.77	27.12	20	200	7403.99	33	23		
93	23.77	27.12	20	210	7418.3	28	13		
94	23.76	27.12	20	220	7535.08	312	14		
95	23.76	27.13	20	230	7475.92	261	17		
96	23.76	27.13	20	240	7506.98	30	11		
97	23.76	27.13	20	250	7493.47	7	12		
98	23.76	27.14	20	260	7557.14	329	19		
99	23.76	27.14	20	270	7557.81	264	13		
100	23.76	27.14	20	280	7537.99	302	8		
101	23.76	27.15	20	290	7485.89	142	12		
102	23.76	27.15	20	300	7557.76	22	19		
103	23.76	27.15	20	310	7426.49	277	2		
104	23.76	27.15	20	320	7505.32	151	8		
105	23.77	27.16	20	330	7509.11	151	16		
106	23.77	27.16	20	340	7396.92	308	19		
107	23.77	27.16	20	350	7436.66	137	14		
108	23.78	27.16	20	360	7484.56	362	12		
109	23.78	27.17	30	10	5673.23	337	6		
110	23.79	27.17	30	20	5823.46	60	10		
111	23.79	27.16	30	30	5962.78	160	7		
112	23.8	27.16	30	40	6167.88	273	15		
113	23.8	27.16	30	50	5982.11	217	19		
114	23.8	27.15	30	60	6059.34	258	24		
115	23.8	27.15	30	70	6210.57	224	22		
116	23.81	27.14	30	80	6269.57	176	20		
117	23.81	27.14	30	90	5977.56	113	21		

(continued)

Table B-1. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3	ppm
118	23.81	27.13	30	100	5919.6	214	14		
119	23.8	27.13	30	110	6124.18	219	19		
120	23.8	27.12	30	120	6152.88	136	8		
121	23.8	27.12	30	130	5671.81	356	1		
122	23.8	27.12	30	140	5809.86	27	21		
123	23.79	27.11	30	150	5566.95	342	9		
124	23.79	27.11	30	160	5697.62	338	10		
125	23.78	27.11	30	170	5712.4	355	14		
126	23.78	27.11	30	180	5819.01	28	8		
127	23.77	27.11	30	190	5391.58	352	10		
128	23.77	27.11	30	200	5638.13	23	19		
129	23.76	27.11	30	210	5691.05	16	10		
130	23.76	27.12	30	220	5562.2	23	17		
131	23.75	27.12	30	230	6251.03	338	11		
132	23.75	27.12	30	240	5773.55	353	14		
133	23.75	27.13	30	250	5653.99	300	9		
134	23.75	27.13	30	260	5692.83	247	14		
135	23.75	27.14	30	270	5786.21	91	10		
136	23.75	27.14	30	280	5763.21	41	12		
137	23.75	27.15	30	290	5990.16	36	17		
138	23.75	27.15	30	300	6038.64	277	11		
139	23.75	27.16	30	310	6049.9	277	12		
140	23.76	27.16	30	320	5359.12	24	17		
141	23.76	27.16	30	330	5909.89	277	13		
142	23.77	27.17	30	340	5684.19	365	23		
143	23.77	27.17	30	350	5680.39	193	12		
144	23.78	27.17	30	360	5646.27	137	13		

Table B2. Offshore 1hr Conc - Source and Receptors are on Platform, 1994 (Vertical Discharge with a Nearby Building)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm		
1	23.78	27.14	5	10	8062.03	4	18	Max Conc at 5m:	8099.8	7.07
2	23.78	27.14	5	20	8095.71	361	8	Max Conc at 10m:	7079.7	6.18
3	23.78	27.14	5	30	7896.82	122	23	Max Conc at 20m:	4270.1	3.73
4	23.78	27.14	5	40	8090.95	104	22	Max Conc at 30m:	2866.8	2.50
5	23.78	27.14	5	50	7999.53	140	18			
6	23.78	27.14	5	60	8000.01	351	19	Avg Conc at 5m:	7983.3	6.97
7	23.78	27.14	5	70	7908.08	132	10	Avg Conc at 10m:	6885.9	6.01
8	23.78	27.14	5	80	7908.28	140	12	Avg Conc at 20m:	4048.2	3.53
9	23.78	27.14	5	90	8057.72	361	11	Avg Conc at 30m:	2679.1	2.34
10	23.78	27.14	5	100	7996.61	356	6			
11	23.78	27.14	5	110	7949.02	354	9	St Dev of Conc at 5m:	6123.2	0.07
12	23.78	27.14	5	120	7908.06	118	3	St Dev of Conc at 10m:	51899.0	0.20
13	23.78	27.14	5	130	8050.57	360	16	St Dev of Conc at 20m:	39341.1	0.17
14	23.78	27.14	5	140	7908.2	17	15	St Dev of Conc at 30m:	21353.8	0.13
15	23.78	27.13	5	150	7908.47	310	14			
16	23.78	27.13	5	160	8028.95	109	17			
17	23.78	27.13	5	170	8055.91	59	18			
18	23.78	27.13	5	180	7908.66	54	12			
19	23.78	27.13	5	190	7908.28	33	11			
20	23.77	27.13	5	200	8097.93	74	12			
21	23.77	27.13	5	210	8099.83	127	8			
22	23.77	27.14	5	220	8055.93	75	12			
23	23.77	27.14	5	230	8095.25	289	16			
24	23.77	27.14	5	240	7908.47	190	15			
25	23.77	27.14	5	250	8001.28	279	24			
26	23.77	27.14	5	260	7896.91	261	19			
27	23.77	27.14	5	270	8083.85	287	18			
28	23.77	27.14	5	280	8063.8	308	20			

(continued)

Table B-2. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
29	23.77	27.14	5	290	7998.86	327	11	
30	23.77	27.14	5	300	7908.47	337	13	
31	23.77	27.14	5	310	* 8100.35	151	9	
32	23.77	27.14	5	320	7864.35	356	18	
33	23.77	27.14	5	330	7908.72	106	13	
34	23.77	27.14	5	340	7897.06	63	6	
35	23.78	27.14	5	350	7919.99	267	18	
36	23.78	27.14	5	360	7974.04	207	14	
37	23.78	27.15	10	10	6991.46	4	18	
38	23.78	27.15	10	20	7039.31	351	18	
39	23.78	27.15	10	30	6394.52	122	23	
40	23.78	27.15	10	40	7042.48	240	13	
41	23.78	27.15	10	50	6941.91	140	18	
42	23.78	27.14	10	60	6938.67	351	19	
43	23.79	27.14	10	70	6762.38	45	19	
44	23.79	27.14	10	80	6760.32	45	19	
45	23.79	27.14	10	90	7000.08	361	11	
46	23.79	27.14	10	100	7079.71	207	12	
47	23.79	27.14	10	110	6985.92	354	9	
48	23.78	27.13	10	120	6890.57	207	15	
49	23.78	27.13	10	130	7076.63	360	16	
50	23.78	27.13	10	140	6404.11	17	15	
51	23.78	27.13	10	150	6959.03	152	10	
52	23.78	27.13	10	160	7078.46	109	17	
53	23.78	27.13	10	170	7075.45	59	18	
54	23.78	27.13	10	180	6665.65	117	18	
55	23.77	27.13	10	190	6404.53	33	11	
56	23.77	27.13	10	200	7024.18	74	12	
57	23.77	27.13	10	210	7061.14	127	8	
58	23.77	27.13	10	220	7075.53	75	12	

(continued)

Table B-2. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
59	23.77	27.13	10	230	7078.41	123	19	
60	23.77	27.13	10	240	6907.86	334	9	
61	23.77	27.14	10	250	7044.43	279	24	
62	23.77	27.14	10	260	6902.3	142	19	
63	23.77	27.14	10	270	7055.28	287	18	
64	23.77	27.14	10	280	6982.49	308	20	
65	23.77	27.14	10	290	6938.19	327	11	
66	23.77	27.14	10	300	6404.72	337	13	
67	23.77	27.15	10	310	7078.93	127	2	
68	23.77	27.15	10	320	6907.42	356	18	
69	23.77	27.15	10	330	6404.73	106	13	
70	23.77	27.15	10	340	6628.25	267	18	
71	23.77	27.15	10	350	6840.35	267	18	
72	23.78	27.15	10	360	7065.99	207	14	
73	23.78	27.16	20	10	4166.66	127	3	
74	23.78	27.16	20	20	4157.58	351	18	
75	23.79	27.16	20	30	3767.45	240	13	
76	23.79	27.15	20	40	4178.55	240	13	
77	23.79	27.15	20	50	3994.78	140	18	
78	23.79	27.15	20	60	3986.72	351	19	
79	23.79	27.15	20	70	3875.01	45	19	
80	23.8	27.14	20	80	3964.15	354	6	
81	23.8	27.14	20	90	4036.5	361	11	
82	23.8	27.14	20	100	4270.05	207	12	
83	23.79	27.13	20	110	4140.08	354	9	
84	23.79	27.13	20	120	4017.27	207	15	
85	23.79	27.13	20	130	4194.73	360	16	
86	23.79	27.12	20	140	3688.07	327	10	
87	23.79	27.12	20	150	4260.23	152	10	
88	23.78	27.12	20	160	4225.11	109	17	

(continued)

Table B-2. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
89	23.78	27.12	20	170	4185.69	59	18	
90	23.78	27.12	20	180	3858.94	117	18	
91	23.77	27.12	20	190	3929.97	333	20	
92	23.77	27.12	20	200	4035.81	74	12	
93	23.77	27.12	20	210	4122.74	78	5	
94	23.76	27.12	20	220	4218.36	5	6	
95	23.76	27.13	20	230	4231.08	123	19	
96	23.76	27.13	20	240	4098.42	78	22	
97	23.76	27.13	20	250	4190.8	279	24	
98	23.76	27.14	20	260	4099.65	78	1	
99	23.76	27.14	20	270	4111.72	287	18	
100	23.76	27.14	20	280	4221.61	19	8	
101	23.76	27.15	20	290	4011.07	61	15	
102	23.76	27.15	20	300	3426.3	127	2	
103	23.76	27.15	20	310	4219.39	127	2	
104	23.76	27.15	20	320	4090.19	356	18	
105	23.77	27.16	20	330	3624.78	229	20	
106	23.77	27.16	20	340	3765.47	267	18	
107	23.77	27.16	20	350	4103.43	165	13	
108	23.78	27.16	20	360	4265.84	207	14	
109	23.78	27.17	30	10	2736.44	127	3	
110	23.79	27.17	30	20	2705.77	351	18	
111	23.79	27.16	30	30	2455.53	110	17	
112	23.8	27.16	30	40	2731.34	240	13	
113	23.8	27.16	30	50	2568.88	123	20	
114	23.8	27.15	30	60	2532.01	351	19	
115	23.8	27.15	30	70	2532.42	360	7	
116	23.81	27.14	30	80	2656.86	360	7	
117	23.81	27.14	30	90	2648.56	18	19	
118	23.81	27.13	30	100	2834.46	207	12	

(continued)

Table B-2. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
119	23.8	27.13	30	110	2703.34	354	9	
120	23.8	27.12	30	120	2583.93	207	15	
121	23.8	27.12	30	130	2829.5	327	10	
122	23.8	27.12	30	140	2493.38	327	10	
123	23.79	27.11	30	150	2866.78	152	10	
124	23.79	27.11	30	160	2817.55	258	18	
125	23.78	27.11	30	170	2728	59	18	
126	23.78	27.11	30	180	2586.05	111	11	
127	23.77	27.11	30	190	2674.74	333	20	
128	23.77	27.11	30	200	2680.69	78	5	
129	23.76	27.11	30	210	2791.01	78	5	
130	23.76	27.12	30	220	2859.19	5	6	
131	23.75	27.12	30	230	2784.69	123	19	
132	23.75	27.12	30	240	2728.43	78	22	
133	23.75	27.13	30	250	2745.94	279	24	
134	23.75	27.13	30	260	2753.66	78	1	
135	23.75	27.14	30	270	2753.47	78	1	
136	23.75	27.14	30	280	2839.51	19	8	
137	23.75	27.15	30	290	2754.88	61	15	
138	23.75	27.15	30	300	2274.39	332	18	
139	23.75	27.16	30	310	2769.56	127	2	
140	23.76	27.16	30	320	2669.28	356	18	
141	23.76	27.16	30	330	2344.96	229	20	
142	23.77	27.17	30	340	2434.22	151	11	
143	23.77	27.17	30	350	2744.57	165	13	
144	23.78	27.17	30	360	2834.17	207	14	
						54	20	
						78	4	

**Table B-3. Offshore 1hr Conc - Source and Receptors are on Platform, 1994
Horizontal Discharge Without a Surrounding Building)**

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm	
1	23.78	27.14	5	10	18587.2	275	19	Max Conc at 5m: 21199.4	18.51
2	23.78	27.14	5	20	21199.4	228	1	Max Conc at 10m: 17326.0	15.13
3	23.78	27.14	5	30	19826.62	229	5	Max Conc at 20m: 9421.9	8.23
4	23.78	27.14	5	40	18748.05	268	10	Max Conc at 30m: 6819.9	5.96
5	23.78	27.14	5	50	18148.25	169	13		
6	23.78	27.14	5	60	20121.06	232	16	Avg Conc at 5m: 19122.4	16.70
7	23.78	27.14	5	70	18940.65	232	16	Avg Conc at 10m: 16466.7	14.38
8	23.78	27.14	5	80	18632.81	219	13	Avg Conc at 20m: 9086.6	7.93
9	23.78	27.14	5	90	19144.69	230	12	Avg Conc at 30m: 6493.7	5.67
10	23.78	27.14	5	100	18605.37	198	20		
11	23.78	27.14	5	110	18826.02	230	11	strd dev of Conc at 5m: 436825.0	0.58
12	23.78	27.14	5	120	19772.95	252	7	strd dev of Conc at 10m: 67072.3	0.23
13	23.78	27.14	5	130	18374.24	263	20	strd dev of Conc at 20m: 24978.5	0.14
14	23.78	27.14	5	140	19034.94	238	11	strd dev of Conc at 30m: 42994.6	0.18
15	23.78	27.13	5	150	19618.28	238	11		
16	23.78	27.13	5	160	19204.78	236	15		
17	23.78	27.13	5	170	19620.42	237	13		
18	23.78	27.13	5	180	19029.25	237	13		
19	23.78	27.13	5	190	18036.94	299	13		
20	23.77	27.13	5	200	18058.08	256	16		
21	23.77	27.13	5	210	18182.72	276	23		
22	23.77	27.14	5	220	18746.82	276	23		
23	23.77	27.14	5	230	18685.98	231	15		
24	23.77	27.14	5	240	19684.63	229	10		
25	23.77	27.14	5	250	19375.32	280	8		
26	23.77	27.14	5	260	19237.84	261	19		
27	23.77	27.14	5	270	19604.61	231	16		

(continued)

Table B-3. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
28	23.77	27.14	5	280	18826.76	290	21	
29	23.77	27.14	5	290	18580.11	263	18	
30	23.77	27.14	5	300	19545.8	231	17	
31	23.77	27.14	5	310	19012.09	246	10	
32	23.77	27.14	5	320	19239.63	232	9	
33	23.77	27.14	5	330	19821.8	232	9	
34	23.77	27.14	5	340	19970.61	226	14	
35	23.78	27.14	5	350	19290.99	270	10	
36	23.78	27.14	5	360	19071.18	230	10	
37	23.78	27.15	10	10	16385.95	279	11	
38	23.78	27.15	10	20	16931.4	228	1	
39	23.78	27.15	10	30	16411.95	262	13	
40	23.78	27.15	10	40	16371.65	304	10	
41	23.78	27.15	10	50	16701.99	264	22	
42	23.78	27.14	10	60	16569.57	240	12	
43	23.79	27.14	10	70	16256.07	291	19	
44	23.79	27.14	10	80	16223.14	219	13	
45	23.79	27.14	10	90	16485.09	222	18	
46	23.79	27.14	10	100	16530.11	204	17	
47	23.79	27.14	10	110	16260.97	15	13	
48	23.78	27.13	10	120	17326.04	229	21	
49	23.78	27.13	10	130	16136.77	181	13	
50	23.78	27.13	10	140	16365.3	245	11	
51	23.78	27.13	10	150	16310.47	305	20	
52	23.78	27.13	10	160	16271.67	300	17	
53	23.78	27.13	10	170	16305.06	237	13	
54	23.78	27.13	10	180	16084.24	80	13	
55	23.77	27.13	10	190	16186.11	299	13	
56	23.77	27.13	10	200	16349.68	303	20	
57	23.77	27.13	10	210	16264.7	190	14	

(continued)

Table B-3. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
58	23.77	27.13	10	220	16453.23	302	3	
59	23.77	27.13	10	230	16358.16	300	15	
60	23.77	27.13	10	240	16459.13	229	10	
61	23.77	27.14	10	250	16549.37	280	8	
62	23.77	27.14	10	260	16739.79	267	19	
63	23.77	27.14	10	270	16620.65	231	16	
64	23.77	27.14	10	280	16561.81	261	18	
65	23.77	27.14	10	290	16313.06	263	18	
66	23.77	27.14	10	300	16428.85	231	17	
67	23.77	27.15	10	310	16742.34	245	12	
68	23.77	27.15	10	320	17050.15	229	6	
69	23.77	27.15	10	330	16523.64	275	15	
70	23.77	27.15	10	340	16615.98	226	14	
71	23.77	27.15	10	350	16468.78	270	10	
72	23.78	27.15	10	360	16187.59	230	10	
73	23.78	27.16	20	10	9184.16	260	6	
74	23.78	27.16	20	20	9097.44	183	9	
75	23.79	27.16	20	30	9197.96	273	17	
76	23.79	27.15	20	40	9288.85	232	8	
77	23.79	27.15	20	50	9109.41	310	16	
78	23.79	27.15	20	60	9255.94	231	20	
79	23.79	27.15	20	70	9234.34	218	21	
80	23.8	27.14	20	80	9151.62	260	18	
81	23.8	27.14	20	90	9235.29	299	22	
82	23.8	27.14	20	100	9421.93	229	23	
83	23.79	27.13	20	110	9211.38	230	20	
84	23.79	27.13	20	120	9101.31	162	2	
85	23.79	27.13	20	130	9065.26	351	15	
86	23.79	27.12	20	140	8960.8	343	23	
87	23.79	27.12	20	150	8687.56	342	9	

(continued)

Table B-3. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
88	23.78	27.12	20	160	8796.96	228	5	
89	23.78	27.12	20	170	9090.76	58	9	
90	23.78	27.12	20	180	9133.8	196	16	
91	23.77	27.12	20	190	9195.84	201	9	
92	23.77	27.12	20	200	8925.76	299	7	
93	23.77	27.12	20	210	9002.73	164	11	
94	23.76	27.12	20	220	8965.48	312	14	
95	23.76	27.13	20	230	9104.1	77	23	
96	23.76	27.13	20	240	9183.1	229	11	
97	23.76	27.13	20	250	9158.15	300	4	
98	23.76	27.14	20	260	9225.23	191	18	
99	23.76	27.14	20	270	9188.89	264	13	
100	23.76	27.14	20	280	9194.09	302	8	
101	23.76	27.15	20	290	8915.97	142	12	
102	23.76	27.15	20	300	9213.49	259	17	
103	23.76	27.15	20	310	8868.59	277	2	
104	23.76	27.15	20	320	8948.7	151	8	
105	23.77	27.16	20	330	8961.37	31	4	
106	23.77	27.16	20	340	9049.57	308	18	
107	23.77	27.16	20	350	8780.2	193	12	
108	23.78	27.16	20	360	9009.87	77	8	
109	23.78	27.17	30	10	6391.64	337	6	
110	23.79	27.17	30	20	6441.83	60	10	
111	23.79	27.16	30	30	6461.99	160	7	
112	23.8	27.16	30	40	6780.72	273	15	
113	23.8	27.16	30	50	6660.61	243	5	
114	23.8	27.15	30	60	6740.75	258	24	
115	23.8	27.15	30	70	6759.19	224	22	
116	23.81	27.14	30	80	6819.91	176	20	
117	23.81	27.14	30	90	6573.94	227	3	

(continued)

Table B-3. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
118	23.81	27.13	30	100	6610.03	219	22	
119	23.8	27.13	30	110	6708.68	219	19	
120	23.8	27.12	30	120	6740.27	136	8	
121	23.8	27.12	30	130	6460.01	10	22	
122	23.8	27.12	30	140	6575.08	6	11	
123	23.79	27.11	30	150	6253.26	40	6	
124	23.79	27.11	30	160	6373.5	338	10	
125	23.78	27.11	30	170	6493.3	225	9	
126	23.78	27.11	30	180	6519.04	28	8	
127	23.77	27.11	30	190	5906.79	352	10	
128	23.77	27.11	30	200	6273.18	23	19	
129	23.76	27.11	30	210	6405.64	16	10	
130	23.76	27.12	30	220	6220.96	23	17	
131	23.75	27.12	30	230	6740.3	338	11	
132	23.75	27.12	30	240	6539.06	353	14	
133	23.75	27.13	30	250	6452.17	300	9	
134	23.75	27.13	30	260	6495.46	247	14	
135	23.75	27.14	30	270	6524.91	229	17	
136	23.75	27.14	30	280	6398.54	41	12	
137	23.75	27.15	30	290	6627.87	338	23	
138	23.75	27.15	30	300	6728.32	277	11	
139	23.75	27.16	30	310	6662.82	277	12	
140	23.76	27.16	30	320	6120.22	327	14	
141	23.76	27.16	30	330	6485.82	277	13	
142	23.77	27.17	30	340	6283.8	365	23	
143	23.77	27.17	30	350	6292.87	193	12	
144	23.78	27.17	30	360	6249.91	137	13	

**Table B-4. Offshore 1hr Conc - Source and Receptors are on Platform, 1994
(Horizontal Discharge with a Nearly Building)**

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm		
1	23.78	27.14	5	10	8068.87	4	18	Max Conc at 5m:	8106.6	7.08
2	23.78	27.14	5	20	8102.55	361	8	Max Conc at 10m:	7085.3	6.19
3	23.78	27.14	5	30	7903.09	191	15	Max Conc at 20m:	4272.5	3.73
4	23.78	27.14	5	40	8097.74	104	22	Max Conc at 30m:	2867.9	2.50
5	23.78	27.14	5	50	8006.3	140	18			
6	23.78	27.14	5	60	8006.79	351	19	Avg Conc at 5m:	7989.9	6.98
7	23.78	27.14	5	70	7914.34	132	10	Avg Conc at 10m:	6891.2	6.02
8	23.78	27.14	5	80	7914.52	140	12	Avg Conc at 20m:	4050.3	3.54
9	23.78	27.14	5	90	8064.52	361	11	Avg Conc at 30m:	2680.0	2.34
10	23.78	27.14	5	100	8003.36	356	6			
11	23.78	27.14	5	110	7955.59	354	9	St Dev of Conc at 5m:	6158.6	0.07
12	23.78	27.14	5	120	7914.25	118	3	St Dev of Conc at 10m:	52135.8	0.20
13	23.78	27.14	5	130	8057.23	360	16	St Dev of Conc at 20m:	39424.5	0.17
14	23.78	27.14	5	140	7914.37	17	15	St Dev of Conc at 30m:	21417.2	0.13
15	23.78	27.13	5	150	7914.73	310	14			
16	23.78	27.13	5	160	8035.5	109	17			
17	23.78	27.13	5	170	8062.6	59	18			
18	23.78	27.13	5	180	7914.89	54	12			
19	23.78	27.13	5	190	7914.52	33	11			
20	23.77	27.13	5	200	8104.8	74	12			
21	23.77	27.13	5	210	8106.59	127	8			
22	23.77	27.14	5	220	8062.62	75	12			
23	23.77	27.14	5	230	8102.11	289	16			
24	23.77	27.14	5	240	7914.75	190	15			
25	23.77	27.14	5	250	8007.95	279	24			
26	23.77	27.14	5	260	7903.25	261	19			

(continued)

Table B-4. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
27	23.77	27.14	5	270	8090.71	287	18	
28	23.77	27.14	5	280	8070.67	308	20	
29	23.77	27.14	5	290	8005.64	327	11	
30	23.77	27.14	5	300	7914.69	337	13	
31	23.77	27.14	5	310	* 8107.25	151	9	
32	23.77	27.14	5	320	7870.85	356	18	
33	23.77	27.14	5	330	7914.92	365	10	
34	23.77	27.14	5	340	7903.25	63	6	
35	23.78	27.14	5	350	7926.81	267	18	
36	23.78	27.14	5	360	7980.49	207	14	
37	23.78	27.15	10	10	6997.01	4	18	
38	23.78	27.15	10	20	7044.94	351	18	
39	23.78	27.15	10	30	6398.53	191	15	
40	23.78	27.15	10	40	7048.18	240	13	
41	23.78	27.15	10	50	6947.41	140	18	
42	23.78	27.14	10	60	6944.18	351	19	
43	23.79	27.14	10	70	6767.75	45	19	
44	23.79	27.14	10	80	6765.68	45	19	
45	23.79	27.14	10	90	7005.63	361	11	
46	23.79	27.14	10	100	7085.32	207	12	
47	23.79	27.14	10	110	6991.48	354	9	
48	23.78	27.13	10	120	6896.11	207	15	
49	23.78	27.13	10	130	7082.27	360	16	
50	23.78	27.13	10	140	6408.05	17	15	
51	23.78	27.13	10	150	6964.26	152	10	
52	23.78	27.13	10	160	7084.06	109	17	
53	23.78	27.13	10	170	7081.1	59	18	
54	23.78	27.13	10	180	6670.91	117	18	
55	23.77	27.13	10	190	6408.52	33	11	
56	23.77	27.13	10	200	7029.76	74	12	

(continued)

Table B-4. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
57	23.77	27.13	10	210	7066.71	127	8	
58	23.77	27.13	10	220	7081.19	75	12	
59	23.77	27.13	10	230	7083.99	123	19	
60	23.77	27.13	10	240	6913.36	334	9	
61	23.77	27.14	10	250	7050.12	279	24	
62	23.77	27.14	10	260	6907.83	142	19	
63	23.77	27.14	10	270	7060.96	287	18	
64	23.77	27.14	10	280	6988.03	308	20	
65	23.77	27.14	10	290	6943.69	327	11	
66	23.77	27.14	10	300	6408.7	337	13	
67	23.77	27.15	10	310	7084.54	127	2	
68	23.77	27.15	10	320	6912.92	356	18	
69	23.77	27.15	10	330	6408.69	365	10	
70	23.77	27.15	10	340	6633.55	267	18	
71	23.77	27.15	10	350	6845.82	267	18	
72	23.78	27.15	10	360	7071.58	207	14	
73	23.78	27.16	20	10	4168.94	127	3	
74	23.78	27.16	20	20	4159.84	351	18	
75	23.79	27.16	20	30	3769.54	240	13	
76	23.79	27.15	20	40	4180.87	240	13	
77	23.79	27.15	20	50	3996.82	140	18	
78	23.79	27.15	20	60	3988.75	351	19	
79	23.79	27.15	20	70	3876.98	45	19	
80	23.8	27.14	20	80	3965.77	354	6	
81	23.8	27.14	20	90	4038.57	361	11	
82	23.8	27.14	20	100	4272.45	207	12	
83	23.79	27.13	20	110	4142.34	354	9	
84	23.79	27.13	20	120	4019.42	207	15	
85	23.79	27.13	20	130	4197.02	360	16	
86	23.79	27.12	20	140	3689.82	327	10	

(continued)

Table B-4. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
87	23.79	27.12	20	150	4262.56	152	10	
88	23.78	27.12	20	160	4227.43	109	17	
89	23.78	27.12	20	170	4187.97	59	18	
90	23.78	27.12	20	180	3860.94	117	18	
91	23.77	27.12	20	190	3931.7	333	20	
92	23.77	27.12	20	200	4037.86	74	12	
93	23.77	27.12	20	210	4124.84	78	5	
94	23.76	27.12	20	220	4220.51	5	6	
95	23.76	27.13	20	230	4233.4	123	19	
96	23.76	27.13	20	240	4100.71	78	22	
97	23.76	27.13	20	250	4193.14	279	24	
98	23.76	27.14	20	260	4101.89	78	1	
99	23.76	27.14	20	270	4113.91	287	18	
100	23.76	27.14	20	280	4223.92	19	8	
101	23.76	27.15	20	290	4012.59	61	15	
102	23.76	27.15	20	300	3428.18	127	2	
103	23.76	27.15	20	310	4221.7	127	2	
104	23.76	27.15	20	320	4092.43	356	18	
105	23.77	27.16	20	330	3625.85	229	20	
106	23.77	27.16	20	340	3767.37	267	18	
107	23.77	27.16	20	350	4105.71	165	13	
108	23.78	27.16	20	360	4268.23	207	14	
109	23.78	27.17	30	10	2737.51	127	3	
110	23.79	27.17	30	20	2706.8	351	18	
111	23.79	27.16	30	30	2455.99	110	17	
112	23.8	27.16	30	40	2732.41	240	13	
113	23.8	27.16	30	50	2569.36	123	20	
114	23.8	27.15	30	60	2532.87	351	19	
115	23.8	27.15	30	70	2533.14	360	7	
116	23.81	27.14	30	80	2657.61	360	7	

(continued)

Table B-4. (continued)

Rec No.	X (km)	Y (km)	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Julian Day	Hour	ug/m3 ppm
117	23.81	27.14	30	90	2649.36	18	19	
118	23.81	27.13	30	100	2835.61	207	12	
119	23.8	27.13	30	110	2704.38	354	9	
120	23.8	27.12	30	120	2584.87	207	15	
121	23.8	27.12	30	130	2830.5	327	10	
122	23.8	27.12	30	140	2494.26	327	10	
123	23.79	27.11	30	150	2867.94	152	10	
124	23.79	27.11	30	160	2818.49	258	18	
125	23.78	27.11	30	170	2729.03	59	18	
126	23.78	27.11	30	180	2586.62	111	11	
127	23.77	27.11	30	190	2675.62	333	20	
128	23.77	27.11	30	200	2681.71	78	5	
129	23.76	27.11	30	210	2792.07	78	5	
130	23.76	27.12	30	220	2860.28	5	6	
131	23.75	27.12	30	230	2785.77	123	19	
132	23.75	27.12	30	240	2729.54	78	22	
133	23.75	27.13	30	250	2747.02	279	24	
134	23.75	27.13	30	260	2754.77	78	1	
135	23.75	27.14	30	270	2754.58	78	1	
136	23.75	27.14	30	280	2840.66	19	8	
137	23.75	27.15	30	290	2755.66	61	15	
138	23.75	27.15	30	300	2274.69	332	18	
139	23.75	27.16	30	310	2770.64	127	2	
140	23.76	27.16	30	320	2670.3	356	18	
141	23.76	27.16	30	330	2345.41	229	20	
142	23.77	27.17	30	340	2434.56	151	11	
143	23.77	27.17	30	350	2745.69	165	13	
144	23.78	27.17	30	360	2835.32	207	14	

**Table B-5. Onshore 1hr Conc - Source and Receptors are Onshore, 1994
(Vertical Discharge with a Nearby Building)**

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3	ppm
1	5	10	8030.3	94081501	Max Conc at 5m:	9.78
2	5	20	8321.6	94081501	Max Conc at 10m:	8.66
3	5	30	8434.0	94081501	Max Conc at 20m:	12.11
4	5	40	8626.2	94081501	Max Conc at 30m:	13.64
5	5	50	8874.8	94081501	Max Conc at 40m:	7.16
6	5	60	9131.3	94081501		
7	5	70	9346.8	94081501	Avg Conc at 5m:	7.97
8	5	80	9479.3	94081501	Avg Conc at 10m:	6.99
9	5	90	9525.2	94072507	Avg Conc at 20m:	8.15
10	5	100	9456.3	94072507	Avg Conc at 30m:	6.73
11	5	110	9286.1	94072507	Avg Conc at 40m:	4.10
12	5	120	9048.1	94072507		
13	5	130	8788.3	94072507	St Dev of Conc at 5m:	0.87
14	5	140	8556.2	94072507	St Dev of Conc at 10m:	0.93
15	5	150	8398.6	94072507	St Dev of Conc at 20m:	2.09
16	5	160	8202.6	94072507	St Dev of Conc at 30m:	3.73
17	5	170	7972.5	94072507	St Dev of Conc at 40m:	1.44
18	5	180	7905.5	94072507		
19	5	190	8030.3	94081501		
20	5	200	8321.6	94081501		
21	5	210	8750.4	94081501		
22	5	220	9280.5	94081501		
23	5	230	9857.2	94081501		
24	5	240	10409.1	94081501		
25	5	250	10856.7	94081501		
26	5	260	11127.7	94081501		
27	5	270	11205.6	94072507		
28	5	280	11065.2	94072507		

(continued)

Table B-5. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
29	5	290	10715.5	94072507	
30	5	300	10215.7	94072507	
31	5	310	9643.4	94072507	
32	5	320	9076.6	94072507	
33	5	330	8580.5	94072507	
34	5	340	8202.6	94072507	
35	5	350	7972.5	94072507	
36	5	360	7905.5	94072507	
37	10	10	9085.0	94081403	
38	10	20	8769.9	94060423	
39	10	30	8106.7	94060423	
40	10	40	7196.5	94060423	
41	10	50	7467.5	94042916	
42	10	60	7244.2	94042916	
43	10	70	6611.6	94042916	
44	10	80	6614.4	94081501	
45	10	90	6722.0	94072507	
46	10	100	6607.3	94091521	
47	10	110	6479.8	94080721	
48	10	120	6402.9	94081205	
49	10	130	6457.6	94111023	
50	10	140	7159.0	94091604	
51	10	150	8014.4	94091604	
52	10	160	8576.3	94091604	
53	10	170	8878.1	94092121	
54	10	180	9312.0	94031224	
55	10	190	8607.6	94010321	
56	10	200	7766.8	94010321	
57	10	210	7631.8	94082823	
58	10	220	7198.2	94082823	
59	10	230	7133.2	94082624	

(continued)

Table B-5. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
60	10	240	8388.3	94081501	
61	10	250	9471.2	94081501	
62	10	260	9857.1	94081501	
63	10	270	9918.4	94081501	
64	10	280	9718.4	94072507	
65	10	290	9226.3	94072507	
66	10	300	8225.4	94072524	
67	10	310	7465.4	94081024	
68	10	320	7480.6	94092804	
69	10	330	8205.6	94092804	
70	10	340	8279.6	94092804	
71	10	350	8793.2	94080620	
72	10	360	9239.4	94041201	
73	20	10	8055.8	94041201	
74	20	20	7661.4	94102503	
75	20	30	9810.0	94042916	
76	20	40	10053.3	94042916	
77	20	50	10841.9	94022417	
78	20	60	11238.6	94070223	
79	20	70	12515.0	94072203	
80	20	80	13351.8	94092020	
81	20	90	13872.6	94081204	
82	20	100	13351.8	94072402	
83	20	110	12511.8	94070401	
84	20	120	11503.8	94062804	
85	20	130	10392.0	94060305	
86	20	140	9299.1	94022824	
87	20	150	8891.1	94092606	
88	20	160	7397.6	94061701	
89	20	170	8452.4	94111023	
90	20	180	8764.7	94091604	

(continued)

Table B-5. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
91	20	190	10329.6	94083124	
92	20	200	11853.4	94010321	
93	20	210	9635.7	94072104	
94	20	220	9521.2	94082823	
95	20	230	7593.7	94082823	
96	20	240	6738.7	94082624	
97	20	250	5050.3	94092821	
98	20	260	5820.8	94081501	
99	20	270	6406.7	94081501	
100	20	280	5679.3	94091022	
101	20	290	4633.4	94070522	
102	20	300	6707.0	94081024	
103	20	310	7665.6	94081024	
104	20	320	9603.4	94092804	
105	20	330	10450.0	94092804	
106	20	340	10594.0	94090620	
107	20	350	10628.3	94060423	
108	20	360	9062.2	94060423	
109	30	10	5269.8	94092819	
110	30	20	9637.0	94092819	
111	30	30	11185.5	94092923	
112	30	40	9663.0	94060624	
113	30	50	11814.8	94022417	
114	30	60	12730.9	94082120	
115	30	70	14370.7	94100521	
116	30	80	15617.2	94092020	
117	30	90	15383.9	94081204	
118	30	100	15617.2	94072402	
119	30	110	14204.4	94080721	
120	30	120	13027.2	94062804	
121	30	130	11620.2	94060305	

(continued)

Table B-5. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
122	30	140	10081.8	94102324	
123	30	150	10907.7	94042901	
124	30	160	9595.0	94051503	
125	30	170	5475.6	94051503	
126	30	180	4406.4	94031224	
127	30	190	5424.8	94111023	
128	30	200	4847.0	94010321	
129	30	210	4929.0	94010321	
130	30	220	3720.4	94082823	
131	30	230	3580.4	94091422	
132	30	240	3833.5	94092821	
133	30	250	3410.6	94072701	
134	30	260	5052.8	94072721	
135	30	270	5923.3	94081501	
136	30	280	5142.1	94091022	
137	30	290	3471.4	94081424	
138	30	300	3495.3	94081105	
139	30	310	3684.6	94081024	
140	30	320	3839.7	94092804	
141	30	330	3913.7	94080620	
142	30	340	4150.3	94042121	
143	30	350	4022.0	94092703	
144	30	360	4383.0	94091424	
145	40	10	3584.4	94042916	
146	40	20	3691.1	94092819	
147	40	30	3702.4	94060624	
148	40	40	5029.8	94031223	
149	40	50	6900.8	94082120	
150	40	60	8048.9	94010420	
151	40	70	7828.1	94100521	
152	40	80	7137.5	94030201	

(continued)

Table B-5. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
153	40	90	5552.1	94081204	
154	40	100	6351.0	94031208	
155	40	110	7763.0	94051501	
156	40	120	8204.8	94071622	
157	40	130	7412.6	94060305	
158	40	140	5546.0	94092701	
159	40	150	3700.9	94090120	
160	40	160	3642.0	94022823	
161	40	170	3481.2	94122401	
162	40	180	3754.5	94031224	
163	40	190	4769.6	94111023	
164	40	200	4152.2	94010321	
165	40	210	4378.7	94010321	
166	40	220	3258.0	94082823	
167	40	230	3227.0	94091422	
168	40	240	3423.1	94092821	
169	40	250	3280.1	94072701	
170	40	260	4344.2	94072721	
171	40	270	5392.8	94082321	
172	40	280	4411.0	94091022	
173	40	290	3186.0	94081424	
174	40	300	3162.0	94081105	
175	40	310	3280.5	94081024	
176	40	320	3359.9	94092804	
177	40	330	3383.0	94080620	
178	40	340	3564.0	94042121	
179	40	350	3467.9	94060324	
180	40	360	3737.2	94091424	

**Table B-6. Onshore 1hr Conc - Source and Receptors are Onshore, 1994
(Horizontal Discharge with a Nearby Building)**

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3	ppm
1	5	10	18313.4	94081501	Max Conc at 5m:	27.7
2	5	20	18977.6	94081501	Max Conc at 10m:	20.8
3	5	30	19234.1	94081501	Max Conc at 20m:	23.5
4	5	40	19672.5	94081501	Max Conc at 30m:	15.5
5	5	50	20239.3	94081501	Max Conc at 40m:	8.5
6	5	60	20824.4	94081501		
7	5	70	21315.8	94081501	Avg Conc at 5m:	19.4
8	5	80	21617.9	94081501	Avg Conc at 10m:	15.4
9	5	90	21670.7	94081501	Avg Conc at 20m:	12.8
10	5	100	21562.2	94091022	Avg Conc at 30m:	8.4
11	5	110	21284.0	94091022	Avg Conc at 40m:	5.2
12	5	120	20809.3	94091022		
13	5	130	20230.6	94091022	St Dev of Conc at 5m:	2.9
14	5	140	19658.7	94091022	St Dev of Conc at 10m:	3.4
15	5	150	19557.8	94010321	St Dev of Conc at 20m:	3.3
16	5	160	20066.0	94010321	St Dev of Conc at 30m:	4.0
17	5	170	20242.1	94010321	St Dev of Conc at 40m:	1.9
18	5	180	30013.9	94091805		
19	5	190	27913.7	94061804		
20	5	200	18979.4	94072721		
21	5	210	19980.5	94072721		
22	5	220	21201.0	94072721		
23	5	230	22512.5	94072721		
24	5	240	23750.2	94072721		
25	5	250	24759.2	94081501		
26	5	260	25377.2	94081501		
27	5	270	25484.7	94081501		
28	5	280	25326.5	94091022		

(continued)

Table B-6. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
29	5	290	24757.9	94091022	
30	5	300	23773.8	94091022	
31	5	310	22534.9	94091022	
32	5	320	21222.1	94091022	
33	5	330	20000.4	94091022	
34	5	340	18998.2	94091022	
35	5	350	27920.7	94062507	
36	5	360	31770.4	94060913	
37	10	10	15451.3	94090620	
38	10	20	13825.7	94090620	
39	10	30	11806.1	94060423	
40	10	40	10480.5	94060423	
41	10	50	10904.1	94072721	
42	10	60	12635.3	94072721	
43	10	70	14147.5	94072721	
44	10	80	15084.5	94081501	
45	10	90	15283.3	94060118	
46	10	100	15091.6	94091022	
47	10	110	14161.5	94091022	
48	10	120	12647.9	94091022	
49	10	130	12522.5	94010321	
50	10	140	14575.6	94010321	
51	10	150	17235.2	94010321	
52	10	160	20261.3	94010321	
53	10	170	22829.6	94010321	
54	10	180	23839.9	94010321	
55	10	190	23309.8	94010321	
56	10	200	21032.9	94010321	
57	10	210	18280.5	94082823	
58	10	220	19262.2	94091422	
59	10	230	19607.4	94053124	

(continued)

Table B-6. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m ³) / (g/s))	Year, Month, Day, & Hour	ug/m ³ ppm
60	10	240	20387.2	94092821	
61	10	250	21505.6	94072721	
62	10	260	22244.4	94081501	
63	10	270	22360.5	94081501	
64	10	280	22203.8	94091022	
65	10	290	21527.5	94091022	
66	10	300	20119.6	94081105	
67	10	310	19797.4	94100822	
68	10	320	19414.0	94091021	
69	10	330	18854.7	94091021	
70	10	340	18368.7	94072421	
71	10	350	17702.8	94072421	
72	10	360	18060.3	94042916	
73	20	10	11211.5	94060423	
74	20	20	9931.3	94011522	
75	20	30	12052.6	94042916	
76	20	40	12351.5	94042916	
77	20	50	13974.1	94022417	
78	20	60	12959.6	94070223	
79	20	70	14235.7	94081206	
80	20	80	15164.8	94092020	
81	20	90	15558.8	94081204	
82	20	100	15187.6	94091520	
83	20	110	14483.3	94010806	
84	20	120	13226.6	94062804	
85	20	130	12083.9	94060305	
86	20	140	11505.5	94112506	
87	20	150	10520.5	94022824	
88	20	160	13000.5	94111023	
89	20	170	15315.0	94111023	
90	20	180	17189.4	94010321	

(continued)

Table B-6. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
91	20	190	23015.6	94010321	
92	20	200	26923.9	94010321	
93	20	210	20560.5	94010321	
94	20	220	19028.2	94102822	
95	20	230	15451.0	94082624	
96	20	240	14059.2	94091202	
97	20	250	10440.0	94091202	
98	20	260	12255.0	94062705	
99	20	270	12575.4	94062705	
100	20	280	10218.4	94062705	
101	20	290	10017.3	94070522	
102	20	300	13816.4	94070522	
103	20	310	15366.0	94062321	
104	20	320	19015.6	94050221	
105	20	330	19863.6	94092804	
106	20	340	18224.8	94052704	
107	20	350	15683.8	94090620	
108	20	360	13197.5	94060423	
109	30	10	5913.7	94092819	
110	30	20	10835.7	94092819	
111	30	30	13149.5	94090520	
112	30	40	12101.0	94022417	
113	30	50	14958.3	94022417	
114	30	60	14779.7	94010420	
115	30	70	16489.1	94100521	
116	30	80	17737.8	94092020	
117	30	90	17264.2	94041904	
118	30	100	17764.5	94091520	
119	30	110	16450.8	94051501	
120	30	120	14978.2	94062804	
121	30	130	13512.2	94060305	

(continued)

Table B-6. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
122	30	140	12470.5	94081824	
123	30	150	13087.5	94120302	
124	30	160	11215.0	94051503	
125	30	170	6362.9	94051503	
126	30	180	5720.7	94111023	
127	30	190	7215.5	94111023	
128	30	200	6690.4	94010321	
129	30	210	6532.1	94010321	
130	30	220	4948.3	94011907	
131	30	230	4782.8	94091422	
132	30	240	4765.6	94080701	
133	30	250	7299.3	94062705	
134	30	260	10431.8	94062705	
135	30	270	10845.6	94062705	
136	30	280	7962.9	94062705	
137	30	290	5089.2	94121509	
138	30	300	5031.5	94070205	
139	30	310	4782.8	94072822	
140	30	320	4903.9	94041820	
141	30	330	4852.6	94072421	
142	30	340	4814.7	94081403	
143	30	350	4803.2	94092703	
144	30	360	5242.5	94042621	
145	40	10	4025.1	94042916	
146	40	20	4142.1	94042916	
147	40	30	4047.2	94090520	
148	40	40	5718.4	94031223	
149	40	50	7992.8	94082120	
150	40	60	9581.5	94010420	
151	40	70	9247.4	94100521	
152	40	80	8476.5	94030201	

(continued)

Table B-6. (continued)

Rec No.	Receptor Distance to the Source (m)	Receptor Direction to the Source (deg)	Conc ((ug/m3) / (g/s))	Year, Month, Day, & Hour	ug/m3 ppm
153	40	90	5337.5	94041904	
154	40	100	7418.6	94031208	
155	40	110	9232.3	94051501	
156	40	120	9614.8	94052801	
157	40	130	8759.1	94060305	
158	40	140	7287.2	94100506	
159	40	150	8655.5	94100506	
160	40	160	6097.6	94100506	
161	40	170	4075.8	94020921	
162	40	180	4346.4	94031501	
163	40	190	5928.1	94111023	
164	40	200	5335.6	94010321	
165	40	210	5325.7	94010321	
166	40	220	4042.3	94011907	
167	40	230	3938.7	94091422	
168	40	240	3951.6	94080701	
169	40	250	5669.0	94062705	
170	40	260	9200.4	94062705	
171	40	270	9704.4	94062705	
172	40	280	6381.3	94062705	
173	40	290	4168.5	94011006	
174	40	300	4472.7	94070205	
175	40	310	3938.7	94072822	
176	40	320	4007.3	94041820	
177	40	330	3896.8	94072421	
178	40	340	3925.4	94042121	
179	40	350	3956.8	94092703	
180	40	360	4349.0	94042621	